Atmospheric composition reanalyses
- Toward Earth System Reanalysis -

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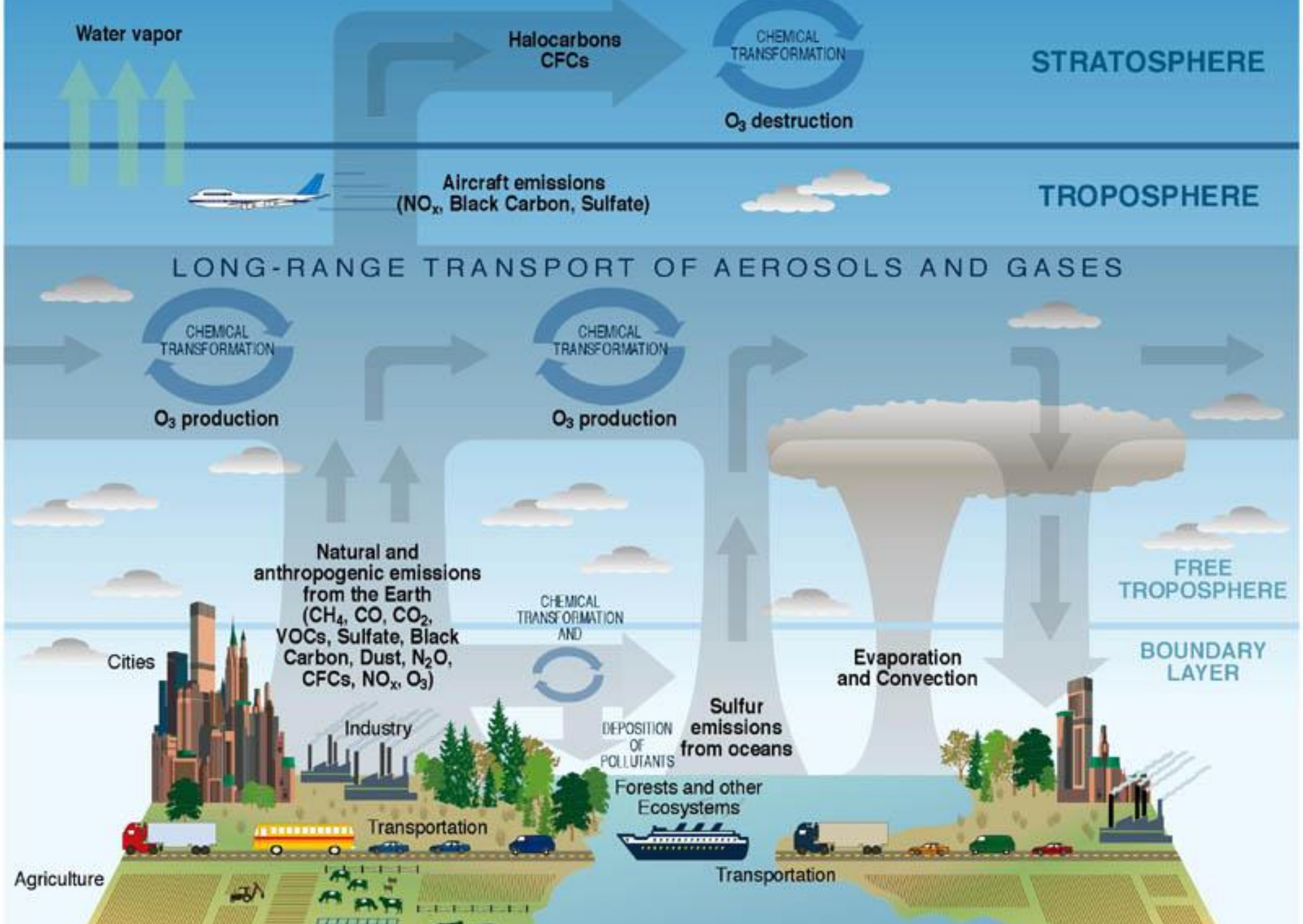
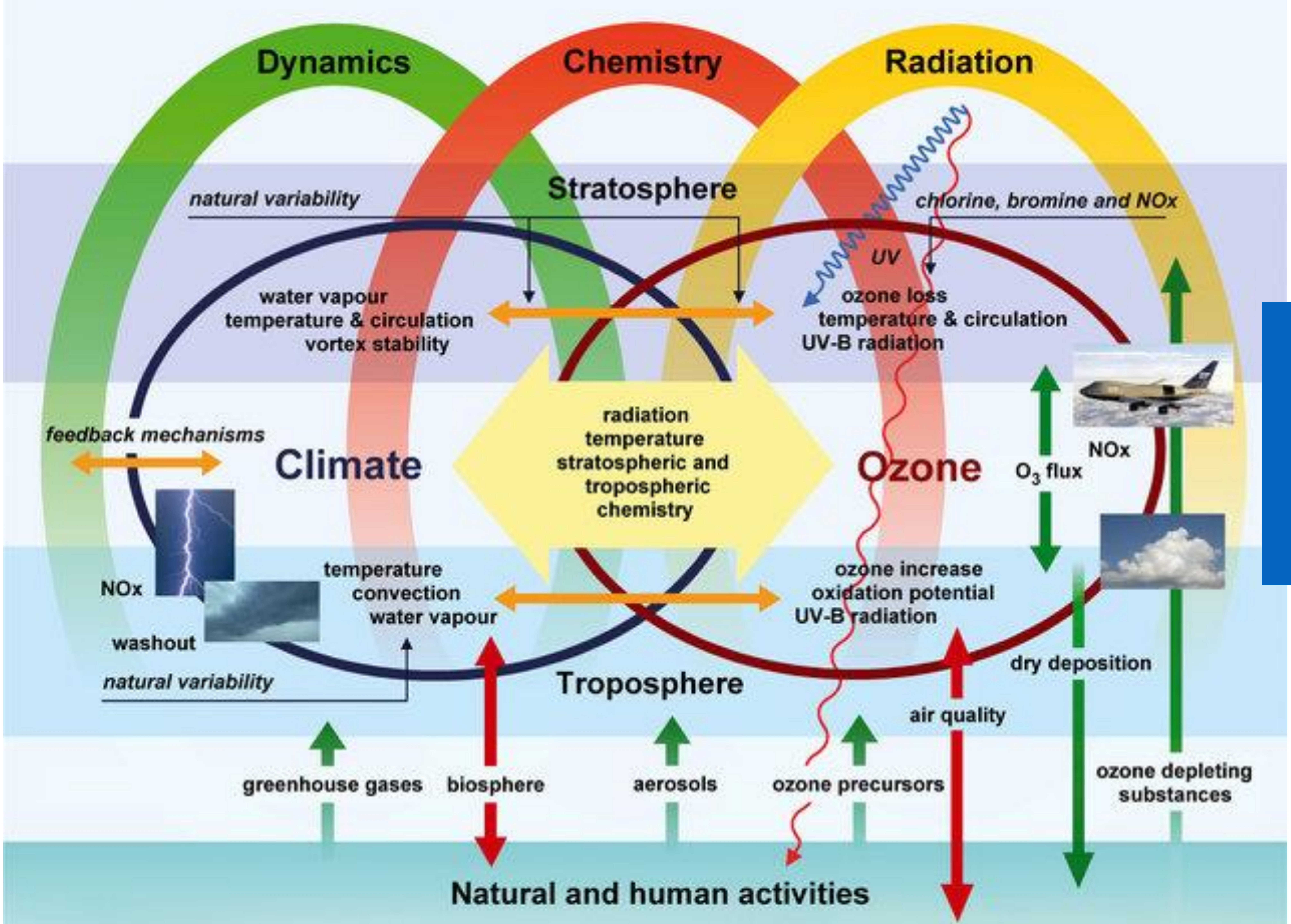

Water vapor
Halocarbons CFCs
CHEMICAL TRANSFORMATION
O_3 destruction
STRATOSPHERE
Aircraft emissions (NO_x, Black Carbon, Sulfate)
TROPOSPHERE
LONG-RANGE TRANSPORT OF AEROSOLS AND GASES
CHEMICAL TRANSFORMATION
O_3 production
CHEMICAL TRANSFORMATION
O_3 production
Natural and anthropogenic emissions from the Earth (CH_4, CO, CO_2, VOCs, Sulfate, Black Carbon, Dust, N_2O, CFCs, NO_x, O_3)
CHEMICAL TRANSFORMATION AND
DEPOSITION OF POLLUTANTS
Sulfur emissions from oceans
Evaporation and Convection
FREE TROPOSPHERE
BOUNDARY LAYER
Cities
Industry
Forests and other Ecosystems
Transportation
Agriculture
Transportation



Comprehensive understanding of coupled systems toward *Earth system reanalysis*

DLR-IMF, after IGACO 2004

Atmospheric composition data assimilation

(1) make best use of all available data from heterogeneous sensors, and

(2) produce chemically and dynamically consistent integrated dataset

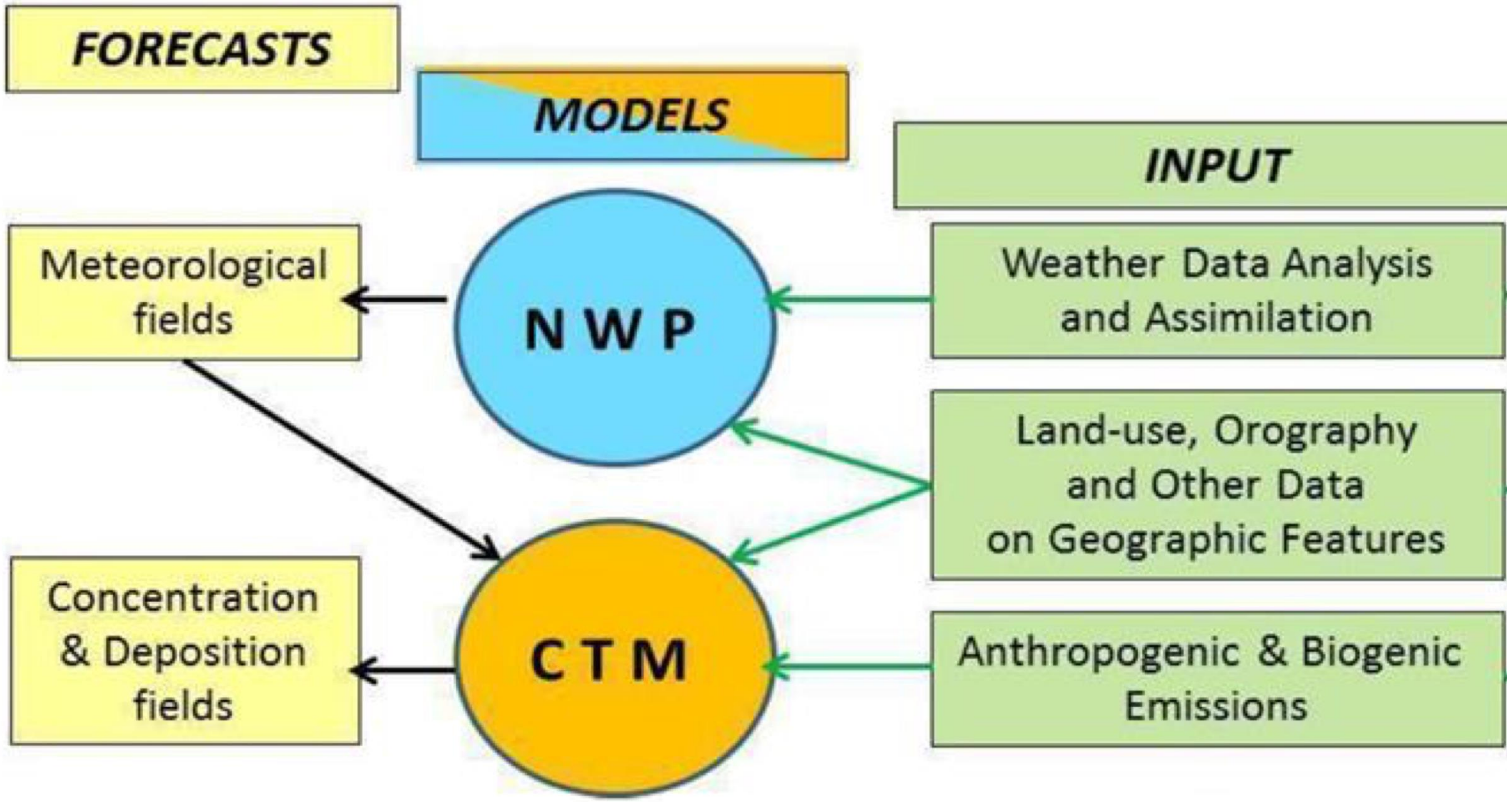
Atmospheric composition data assimilation

Atmospheric composition only

Chemical transport model (CTM)

Coupled with NWP

Coupled chemistry meteorology models (CCMM)



Strato ozone → Temp & wind

AOD → Radiation

Atmospheric composition

Observations

Stratospheric ozone in meteorological reanalyses

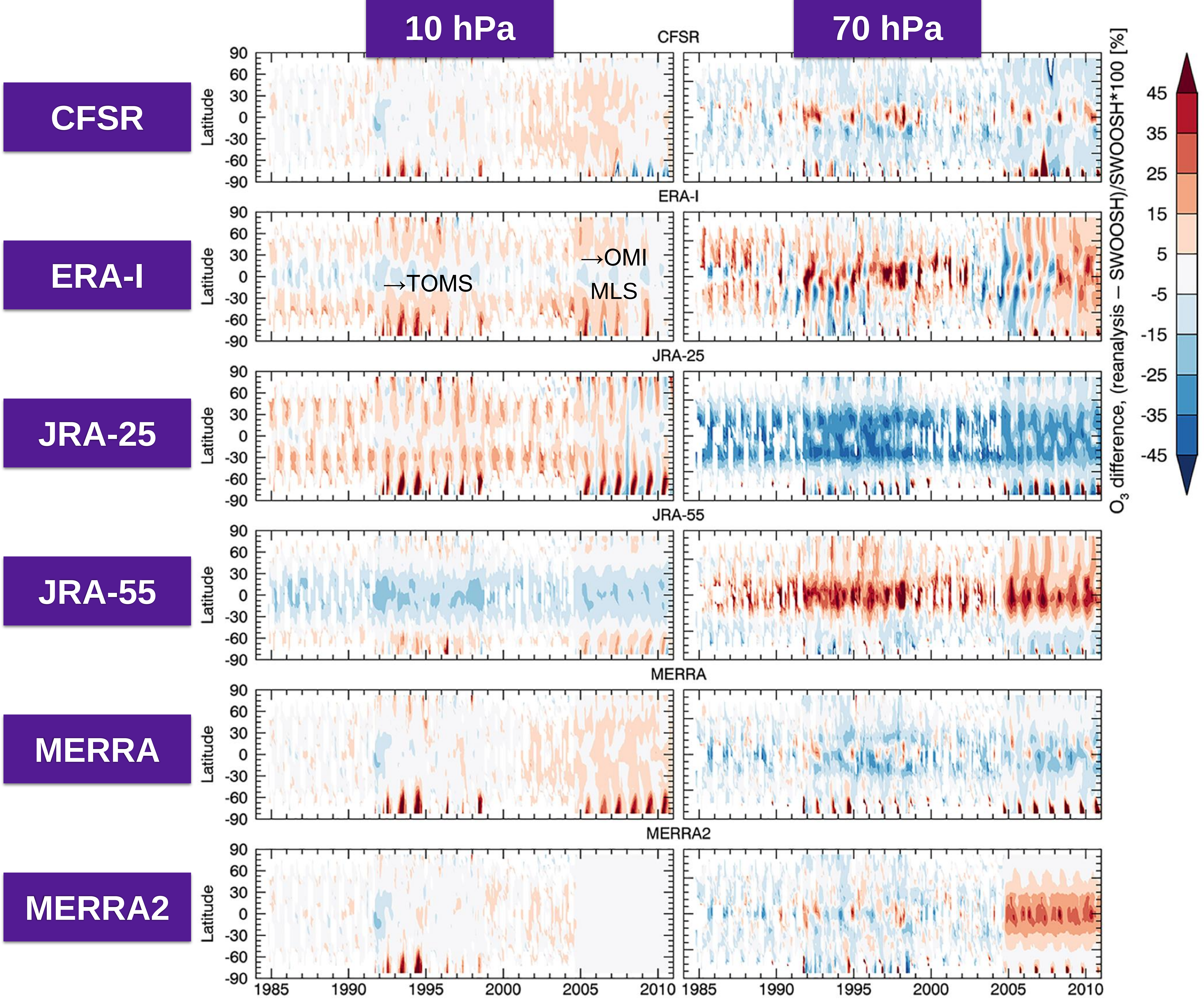
Table 1. Key characteristics of ozone treatment in reanalyses.

Coupled with NPW

Reanalysis	Primary TCO data sources	Vertical profile data sources	Stratospheric O_3 used in radiative transfer	Stratospheric O_3 treatment	Photochemical parameterization
NCEP R1	None	None	Climatology	None	None
NCEP R2	None	None	Climatology	None	None
CFSR	SBUV	SBUV	Analyzed	Prognostic	CHEM2D-OPP
ERA-40	TOMS	SBUV	Climatology	Prognostic	CD86
ERA-I	Same as ERA-40	SBUV, GOME, MLS, MIPAS	Same as ERA-40	Same as ERA-40	Same as ERA-40
JRA-25	TOMS (1979–2004)* OMI (2004–)	Nudging to climatological profile	Daily values from offline CTM	Daily values from offline CTM	Shibata et al. (2005)
JRA-55	Same as JRA-25	None	Daily values from updated offline CTM	Daily values from updated offline CTM	Shibata et al. (2005)
MERRA	SBUV	SBUV	Analyzed	Prognostic	Stajner et al. (2008)
MERRA-2	SBUV (1980–9/2004) OMI (9/2004–)	SBUV, MLS	Same as MERRA	Same as MERRA	Same as MERRA

Davis et al, 2017

Latitude–time evolution of relative differences between ozone in meteorological reanalyses and the merged SWOOSH ozone record.

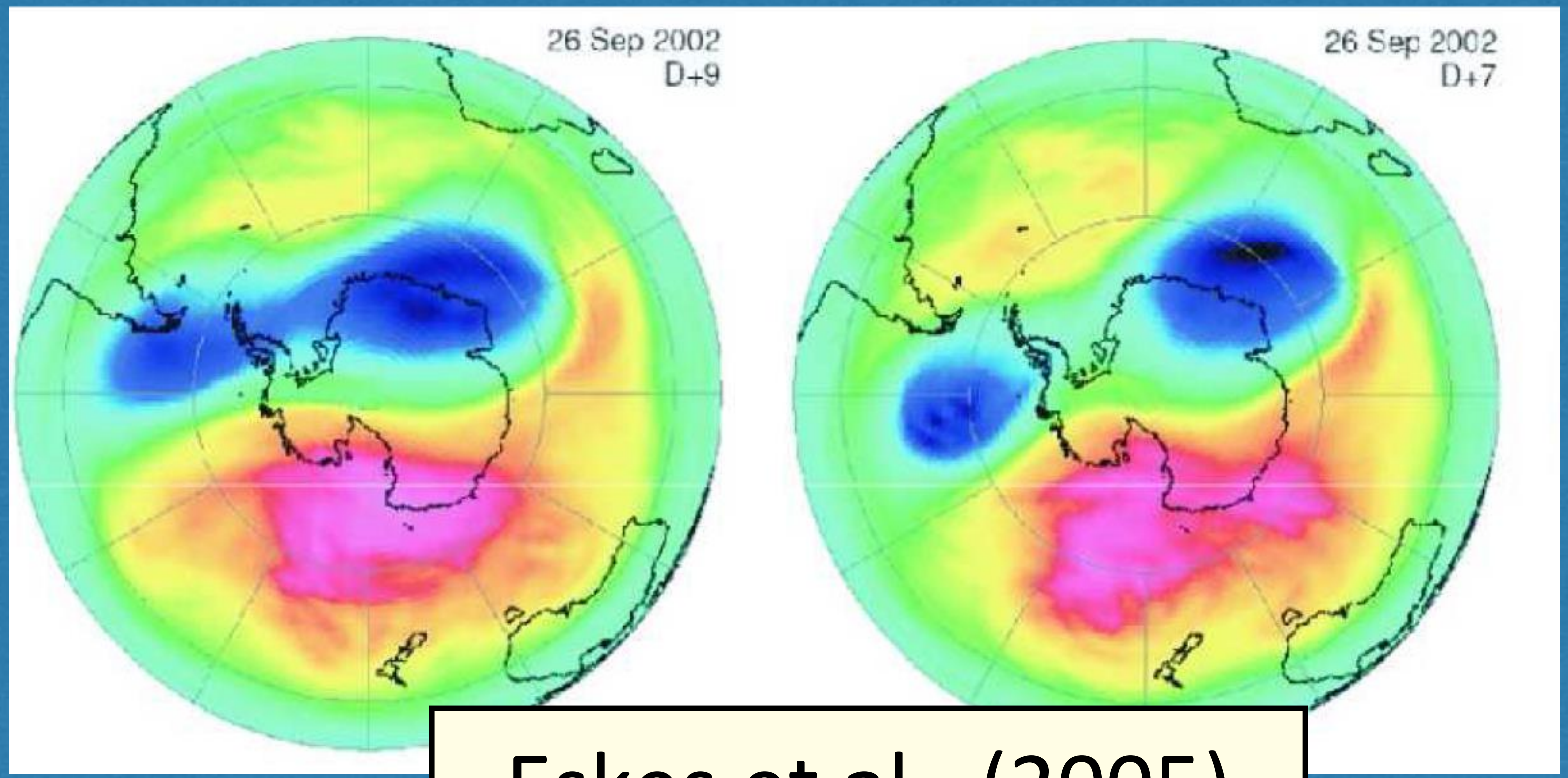


- Relative errors: 10-30 %
- Troposphere: larger errors
- Consistent long-term record is still challenging

Davis et al., 2017

Middle atmosphere

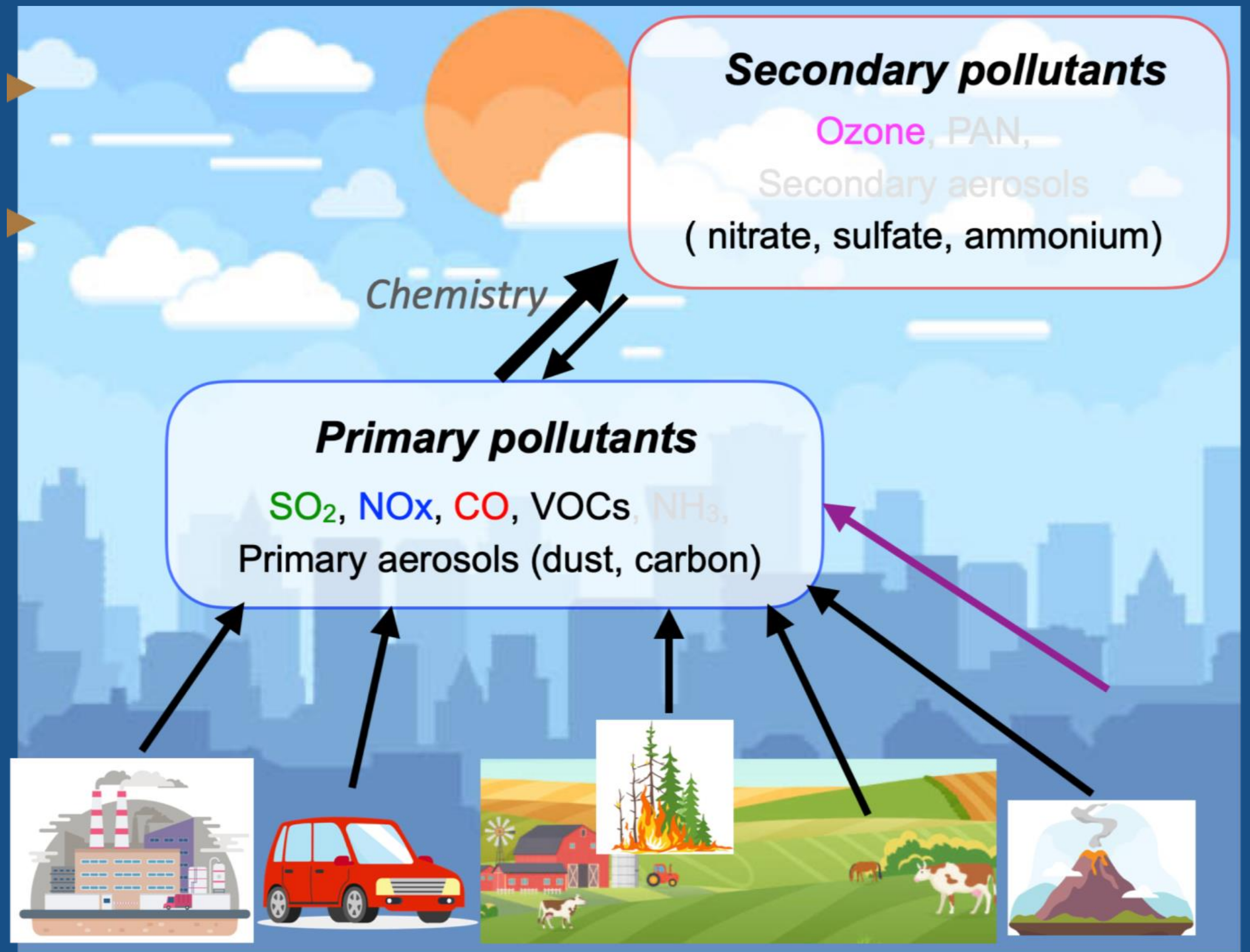
Polavarapu et al. (2005)
Lahoz et al. (2007)



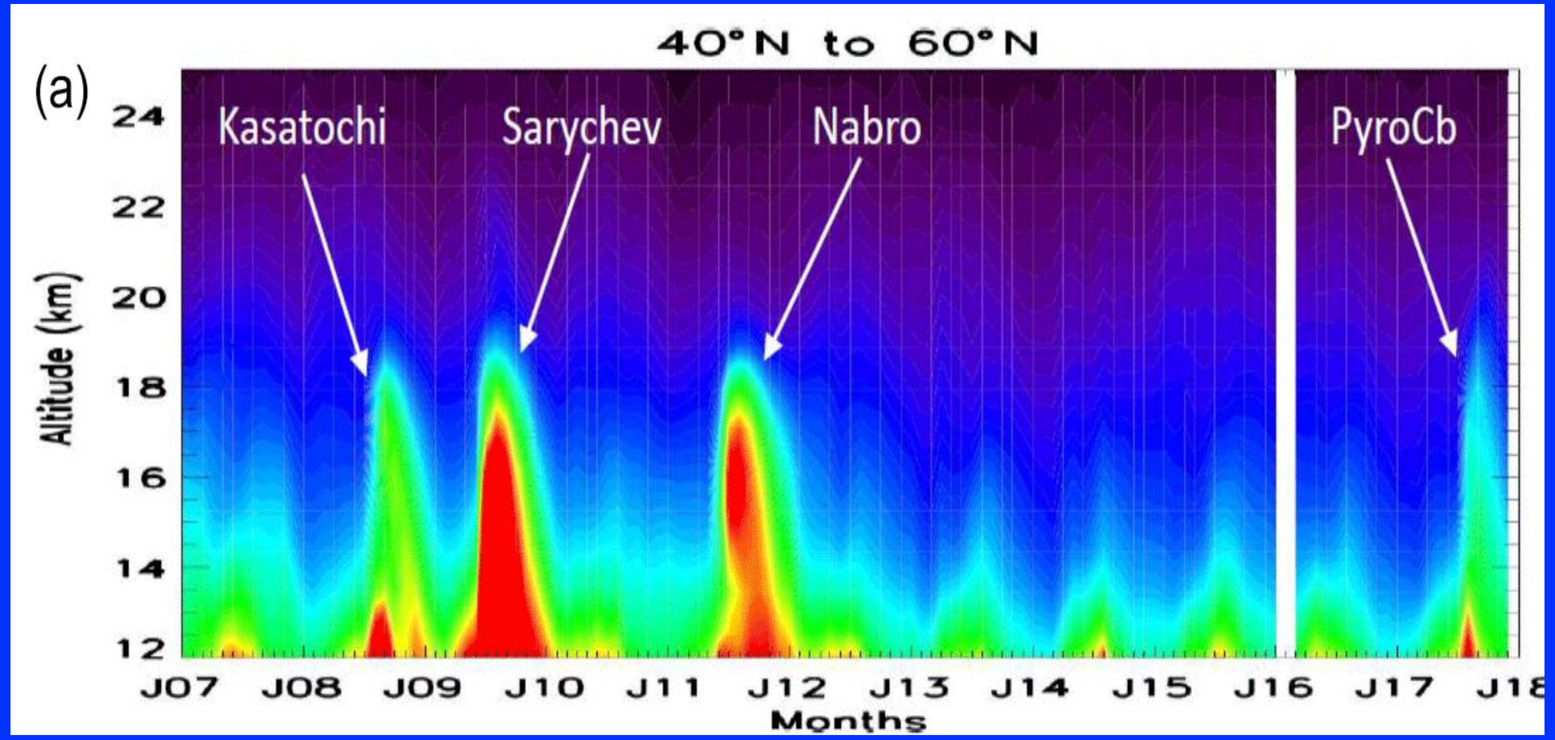
Eskes et al., (2005)

- Ozone hole
- UV monitoring / forecasting
- Radiative forcing
- Middle atmosphere dynamics / chemistry

AC only



- Climate model inputs
- Satellite data validation
- Radiative forcing
- Emission inversion / scenario evaluation
- Air quality monitoring / forecasting
- Extension to non-observed species

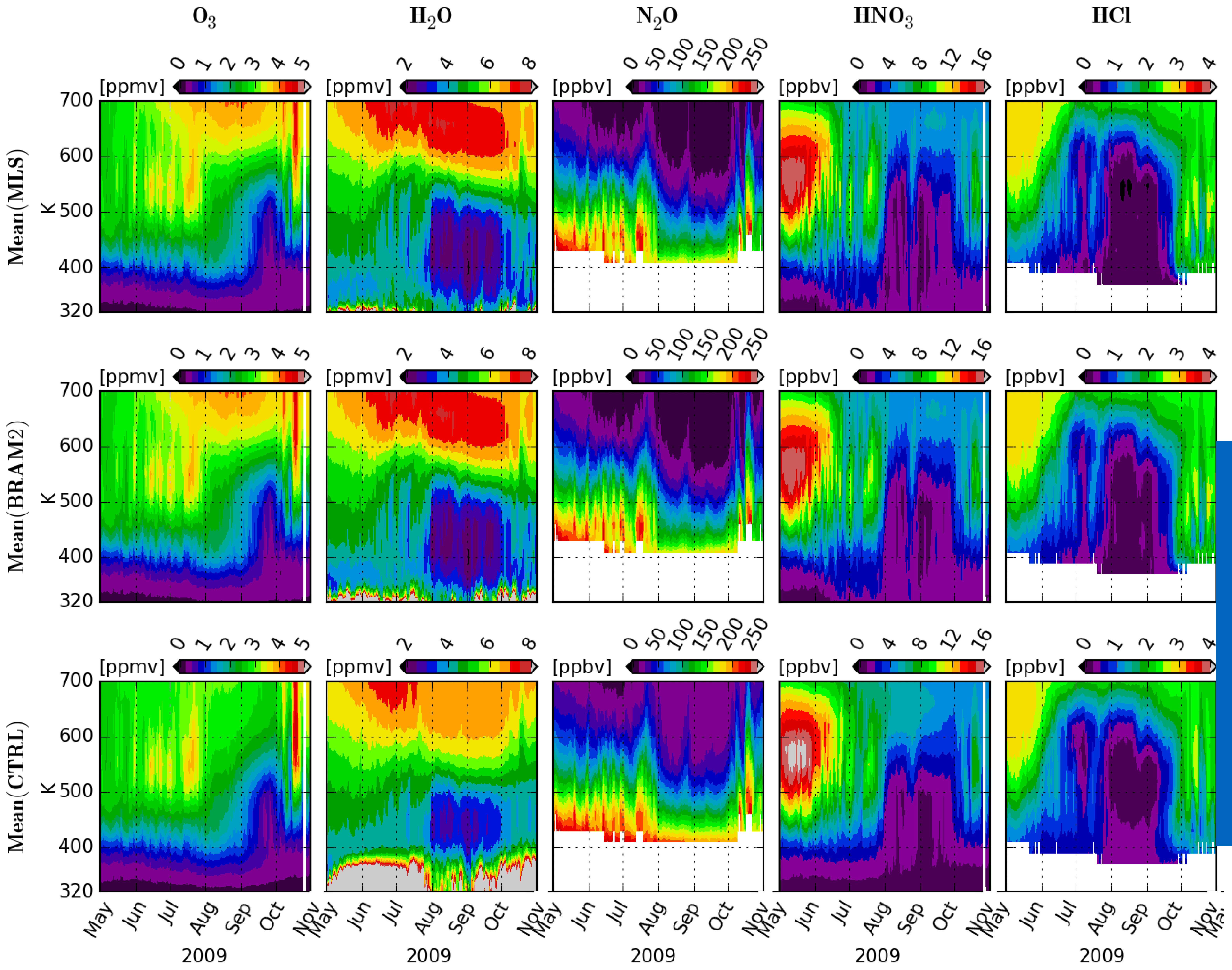


Troposphere: Trace gas

Bocquet et al. (2015)

Troposphere: Aerosols

Chemical reanalysis for the middle atmosphere



Middle atmosphere

MLS chemical reanalysis using Belgian Assimilation System for Chemical ObsErvations (BASCOE)

Provide baseline information to evaluate

(1) chemistry-climate models

(2) bias in independent measurements

and to inform

(3) the stratosphere to troposphere influence

Errera et al, 2019

Tropospheric ozone reanalyses considered in IGAC TOAR-2

Reanalysis system	Grid	Resolution	Period	Strato/Column ozone (Assimilated measurements)	Tropo ozone (Assimilated measurements)	Precursors (Assimilated measurements)	Surface (Assimilated measurements)	Scheme
IASI-R (E. Emili)	GLOBAL, 0.1-1000 hPa	2° x 2°		MLS	IASI			3D-Var
CAMSRA (A. Inness)	GLOBAL	T255, available at 0.75° x 0.75°	-2003	SBUV, OMI, MLS, GOME2, SCIAMACHY, MIPAS, TROPOMI, OMPS		CO, NO2		4D-Var
RAQMS (B. Pierce)	GLOBAL, 0-60km	1° x 1°		OMI cloud cleared, MLS	OMI cloud cleared	MOPITT CO, OMI NO2		3D-Var
GEOS-C								-Var
TCR2 (								nKF
CAQRA (X. Tang)	REGIONAL (CHINA)	15 km x 15 km	-2013			MOPITT CO, OMI NO2	China	EnKF
CMAQ-GSI (R. Kumar)	REGIONAL (US)	12 km x 12 km	2005-2018			MOPITT CO		3D-Var

IGAC Tropospheric Ozone Assessment Report Phase-2 (TOAR-2)

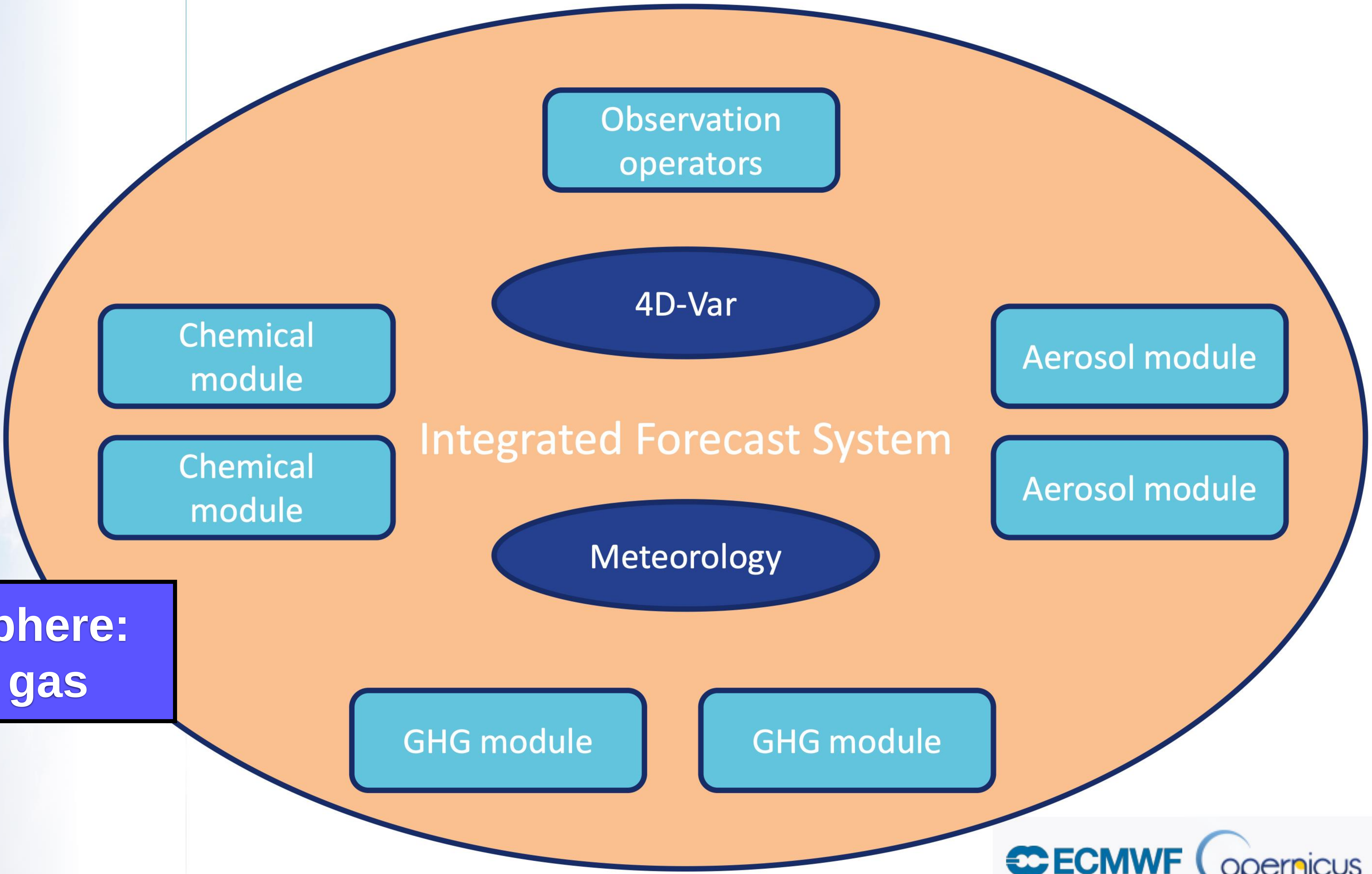
Chemical reanalysis WG

- *Do they agree/disagree with each other and with independent observations?*
- *What is the relative importance of assimilated measurements to improve ozone?*

Troposphere: Trace gas

Global system – ECMWF's IFS

Atmosphere Monitoring



Troposphere: Trace gas

ECMWF Copernicus Europe's eyes on Earth European Commission

Near-real-time satellite data usage

Species	**Instruments**
Global system	
O_3	**OMI**, **SBUV-2**, **GOME-2**, **MLS**, **TROPOMI**, **OMPS,** IASI
CO	**IASI**, **MOPITT**, **TROPOMI**
NO_2	**OMI**, **GOME-2**, **TROPOMI**
SO_2	**OMI**, **GOME-2**, **TROPOMI,** IASI
Aerosol	**MODIS**, **PMAp,** VIIRS, SLSTR, SEVIRI
CO_2	**GOSAT**, **OCO-2**
CH_4	**GOSAT**, **IASI**, **TROPOMI**
GFAS: Fire Radiative Power **Assimilated** **Monitored** Future	**MODIS**, GOES-E/W*, **SEVIRI*,** SLSTR, **VIIRS**, HIMAWARI-8*

*Geostationary platform

A wide-range of atmospheric composition satellite observations are assimilated in the IFS to produce daily analyses.

Control runs (with no data assimilated) and forecasts (initialised from analyses) are also produced in CAMS.

CAMS data used for field campaign planning and evaluating special events.

Composition data additional to thousands of assimilated meteorological data.

MOMO-Chem (Multi-mOdel Multi-cOnstituent Chemical) Data Assimilation System

MLS

TES

OMI

MOPITT

AIRS

SCIAMACHY

GOME-2

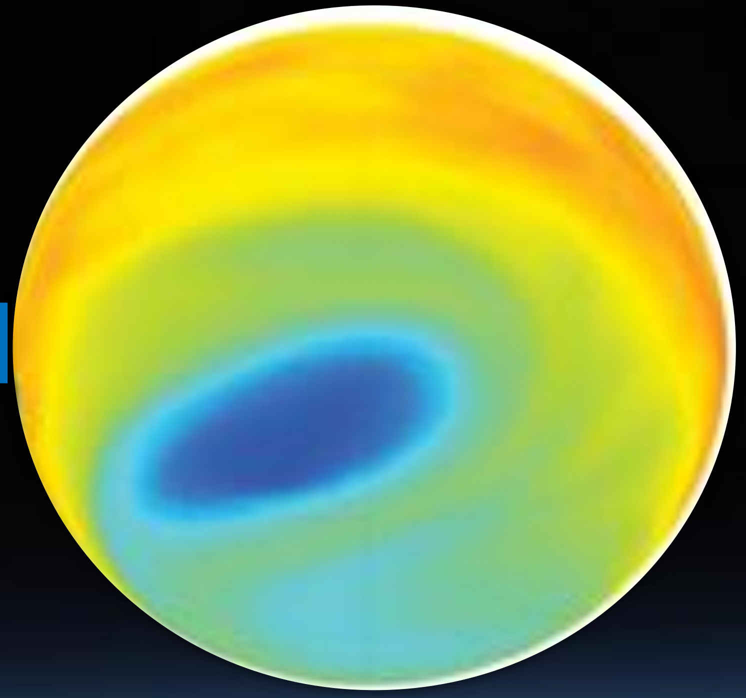
TROPOMI

Satellite Observations Assimilated in MOMO-Chem

Satellite

(O3, CO, NO_2, HNO_3, CO)

Data Assimilation



Physical model

(4 models)

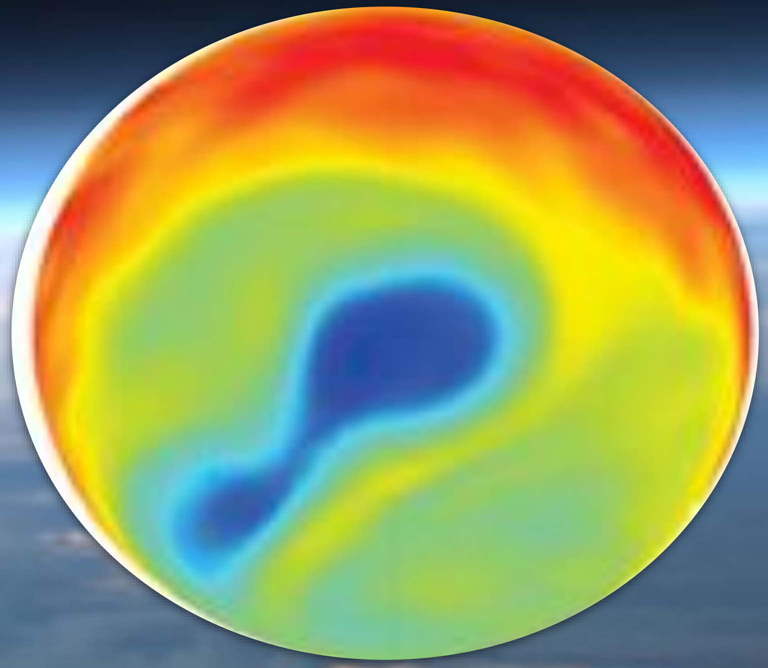
Models Used for Assimilation

CHASER Chemistry Climate Model

MIROC-ESM

TCR

GEOS-Chem



Validation against in-situ & aircraft measurements

DISCOVER-AQ

KORUS-AQ

SEAC4RS

INTEX-B

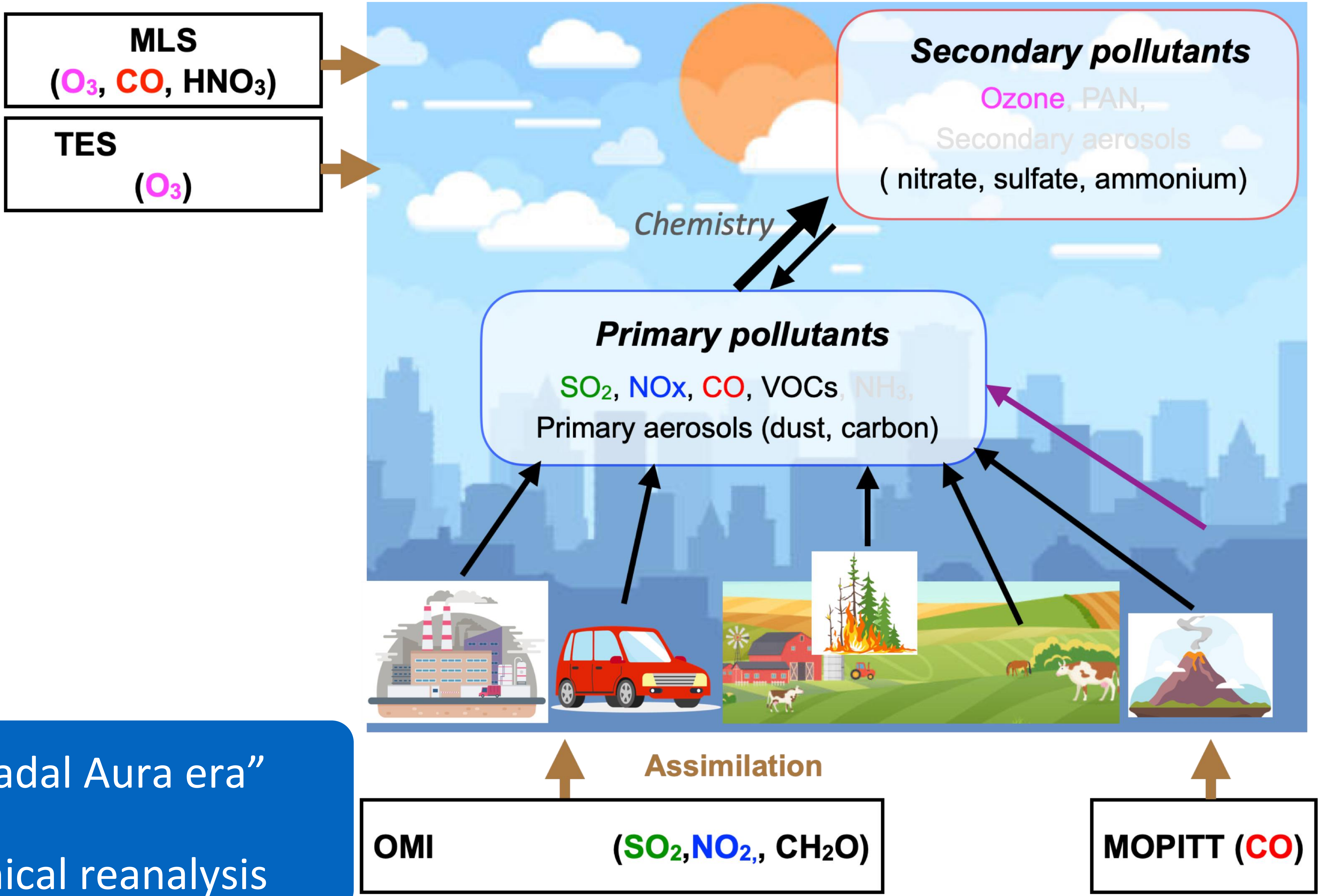
SHADOZ

ATom

Tropospheric Chemical Reanalysis

- 18 years (2005-present), two-hourly, global, chemical concentrations of 35 species
- Anthropogenic, biogenic, biomass burning, and lightning emissions (NOx, CO, SO_2)
- Used in various science applications, including validation of NASA satellite products
- Able to support OSSE activities in support of mission formulation

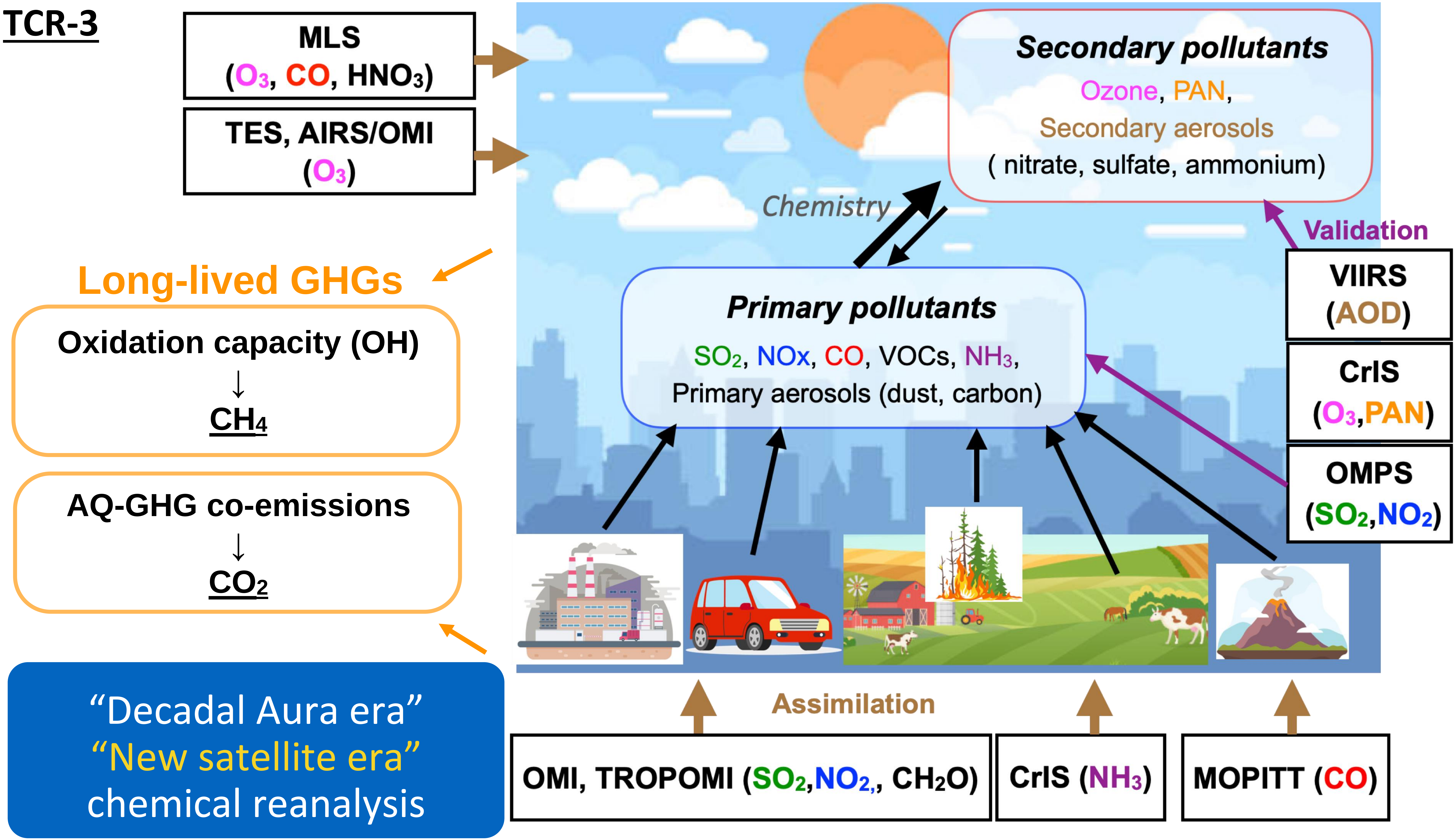
TCR-2



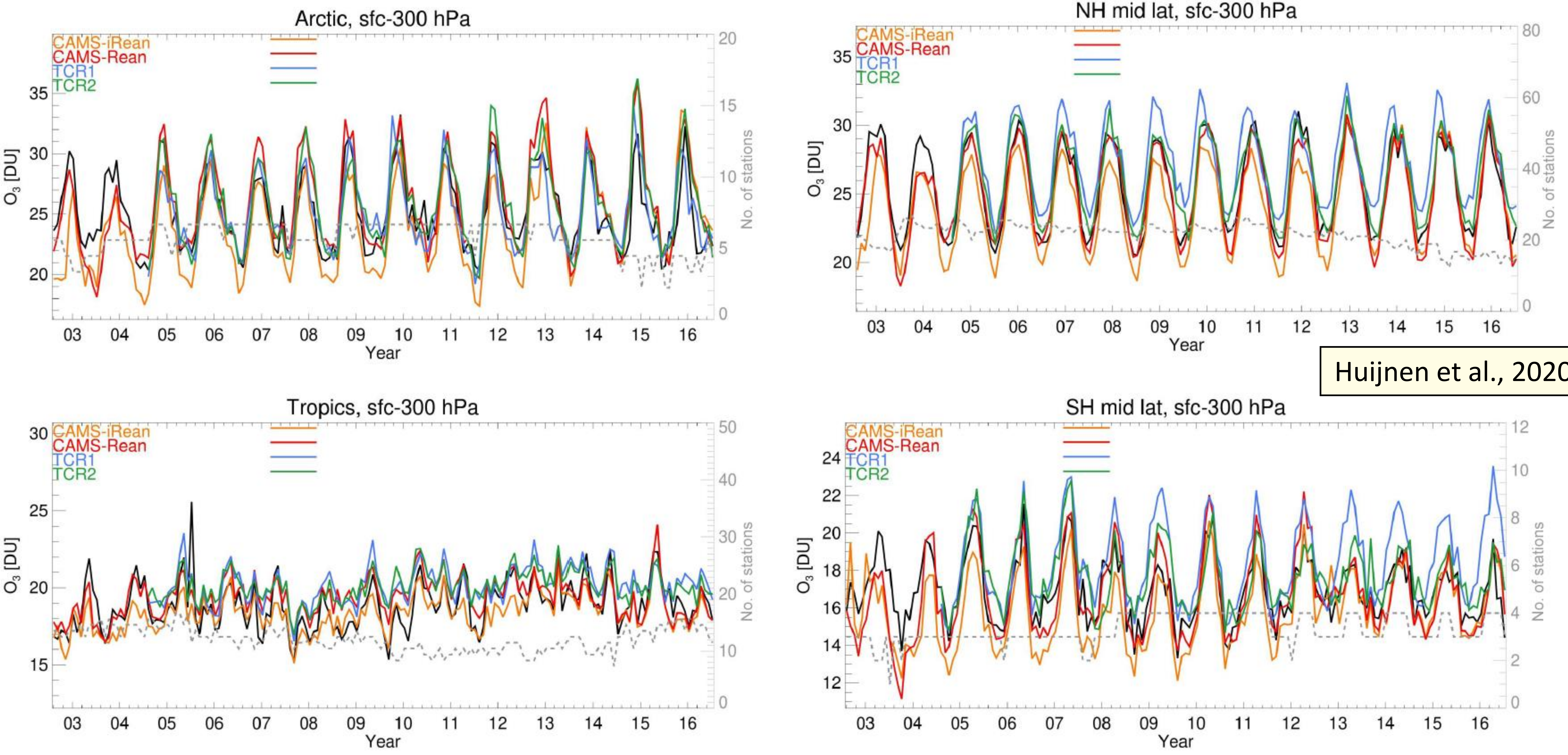
"Decadal Aura era"

chemical reanalysis

TCR-3


MLS
(O_3, CO, HNO_3)
TES, AIRS/OMI
(O_3)
Long-lived GHGs
Oxidation capacity (OH)
↓
CH_4
AQ-GHG co-emissions
↓
CO_2
Secondary pollutants
Ozone, PAN,
Secondary aerosols
(nitrate, sulfate, ammonium)
Chemistry
Validation
Primary pollutants
SO_2, NOx, CO, VOCs, NH_3,
Primary aerosols (dust, carbon)
VIIRS
(AOD)
CrIS
(O_3,PAN)
OMPS
(SO_2,NO_2)
Assimilation
OMI, TROPOMI (SO_2,NO_2,, CH_2O)
CrIS (NH_3)
MOPITT (CO)
"Decadal Aura era"
"New satellite era"
chemical reanalysis

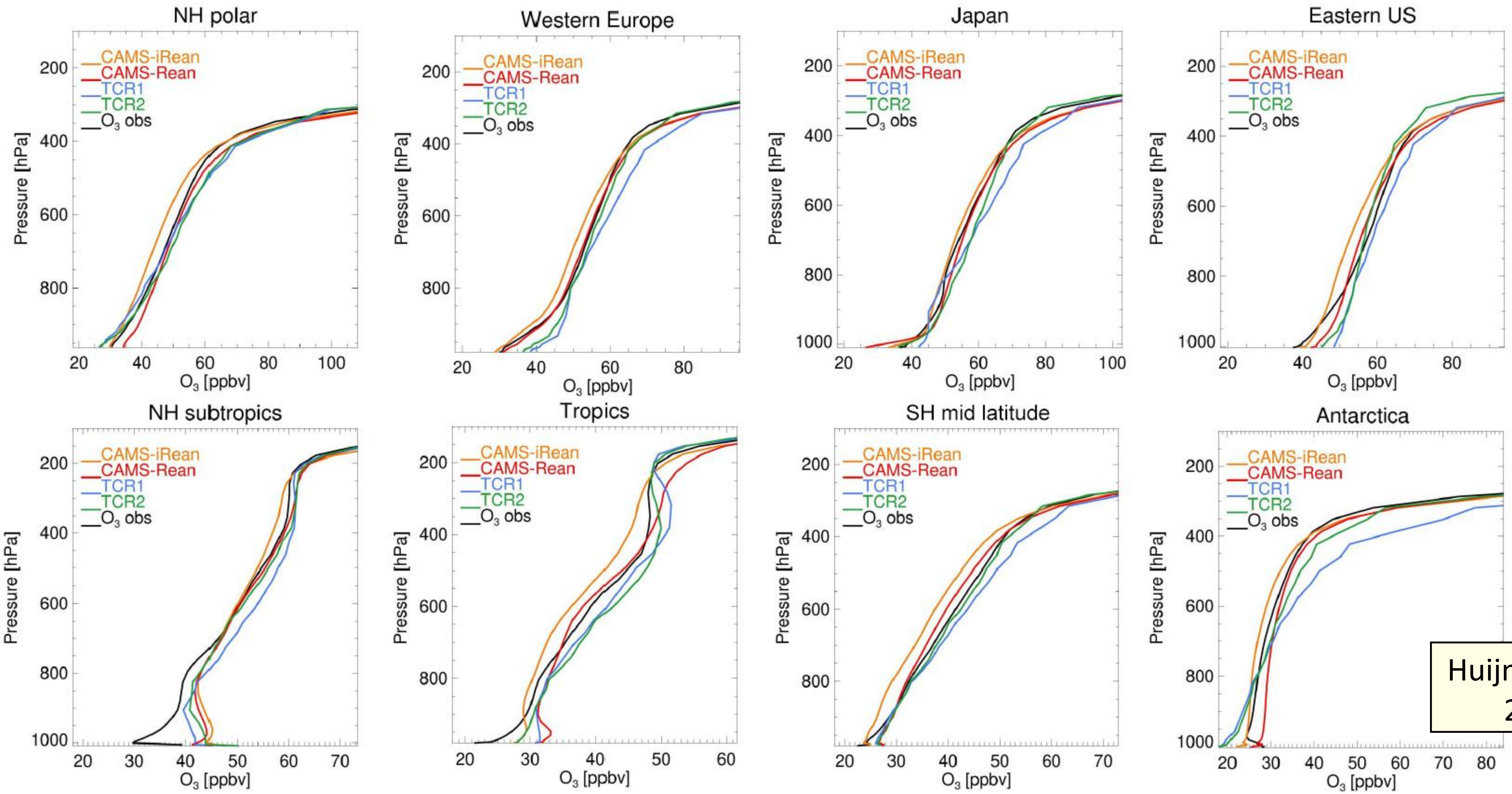
Chemical reanalysis inter-comparisons: CAMS & TCR



Huijnen et al., 2020

Improvements in both forecast model and DA led to better agreements with independent obs

Chemical reanalysis inter-comparisons: CAMS & TCR



Huijnen et al. 2020

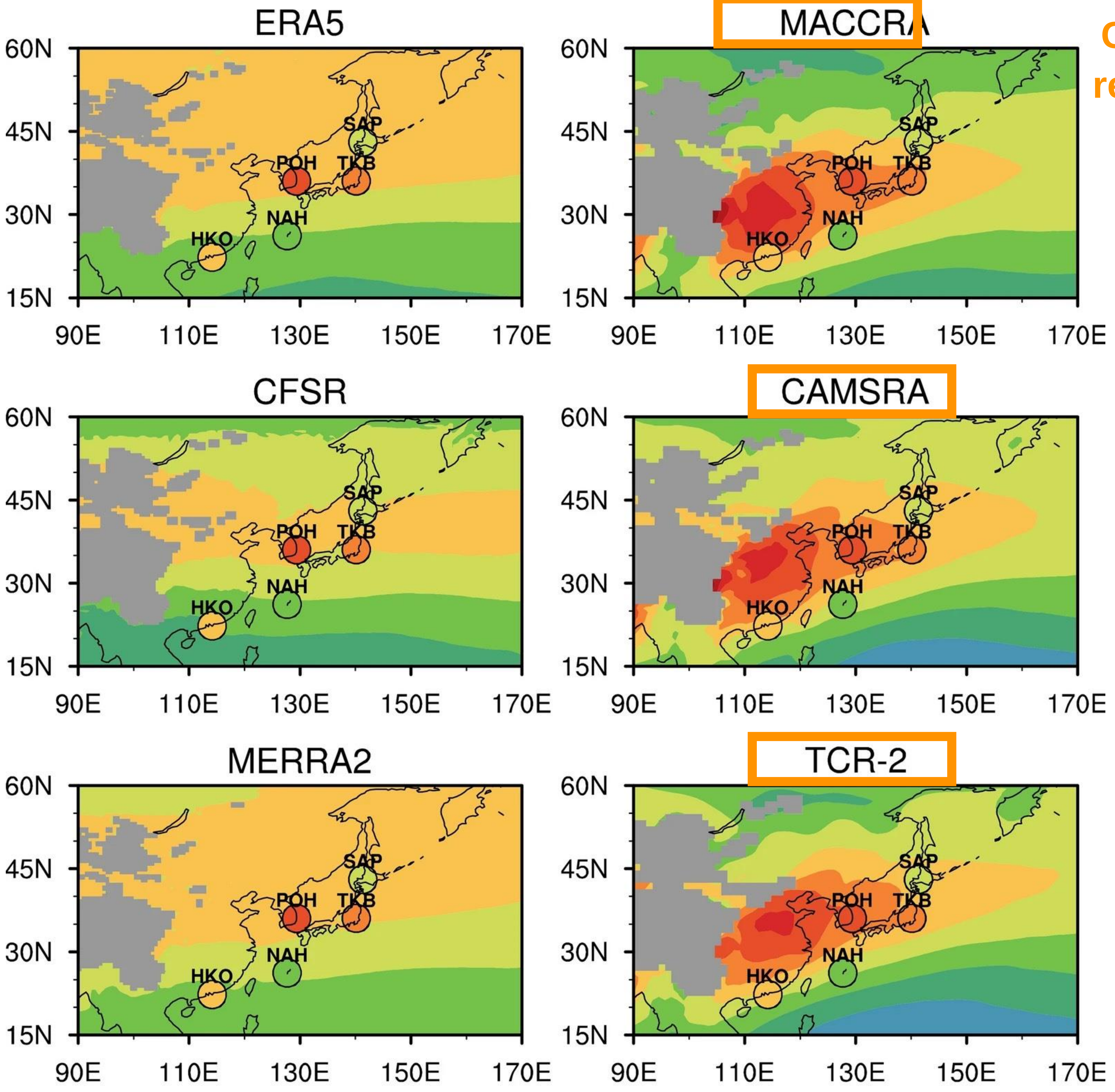
Remaining errors in the tropics and near the surface

Need to improve model performance, incl. spatial resolution, increasing obs, incl. surface obs, and DA

Ozone reanalysis inter-comparisons

Met reanalysis

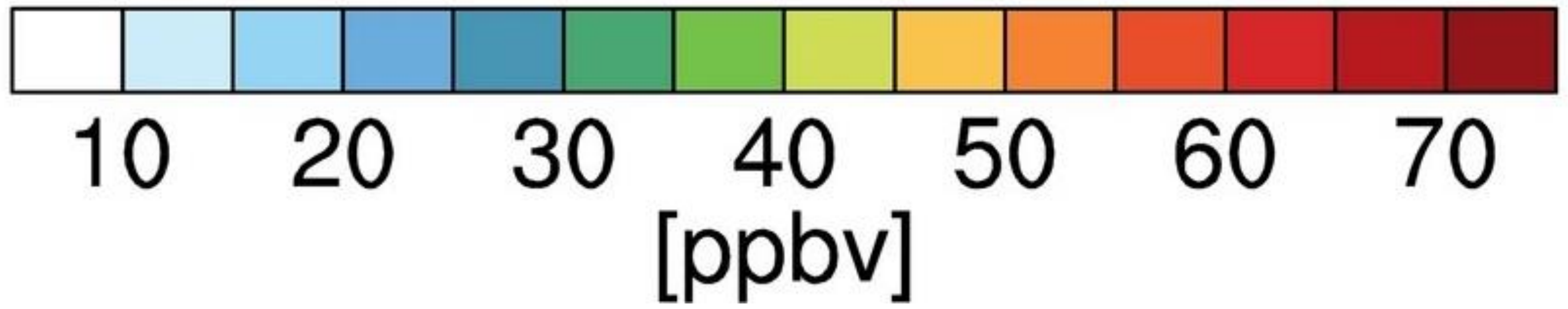
Chemical reanalysis



850 hPa ozone over East Asia, validated against ozonesonde measurements

- Controlled by emissions, transport from China and Pacific
- The chemical reanalyses are useful for AQ research
- The met reanalyses do not capture the major spatial gradients

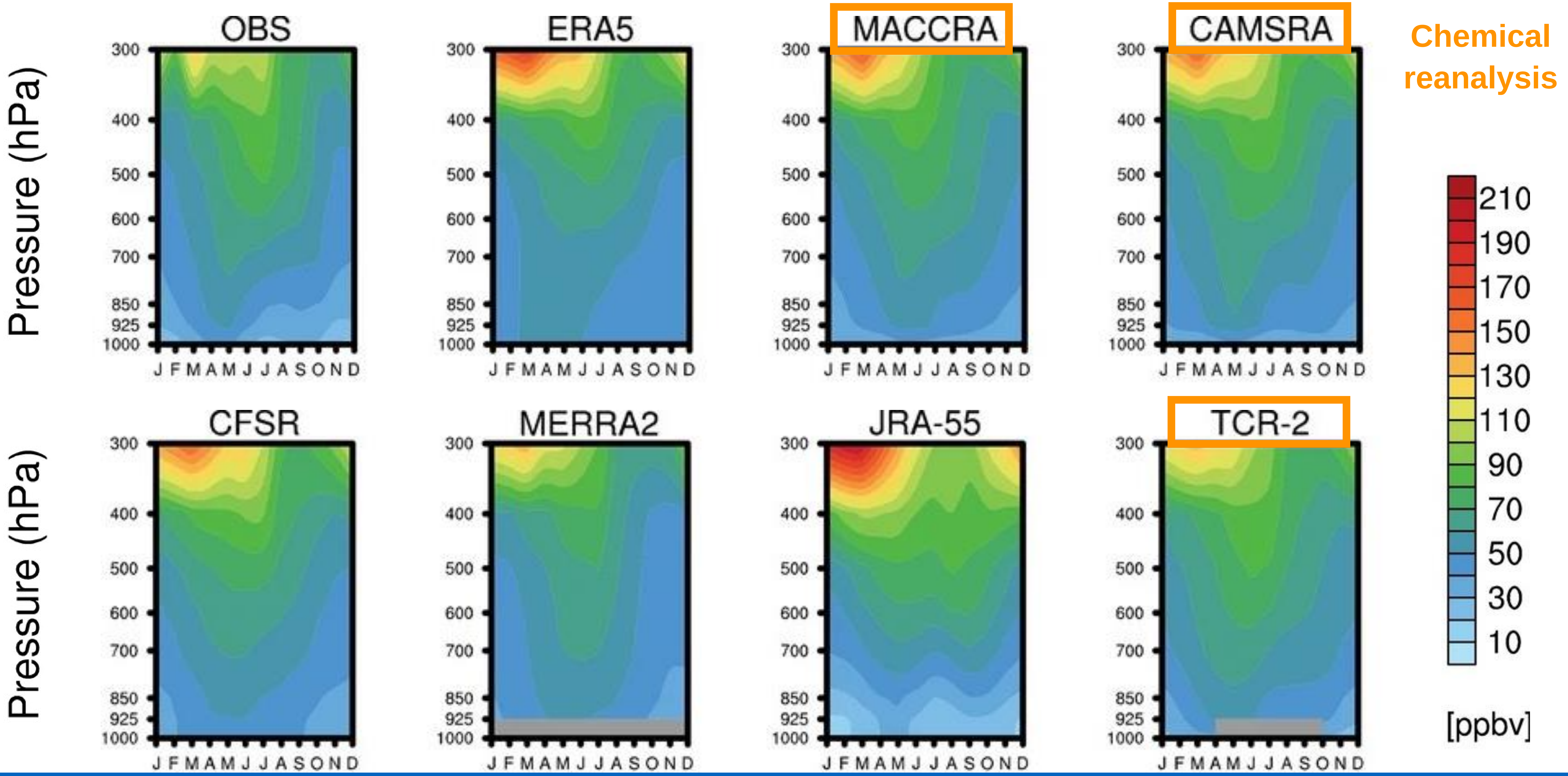
Park et al, 2020



Ozone reanalysis inter-comparisons

Seasonal and vertical distribution of ozone over Sapporo, Japan

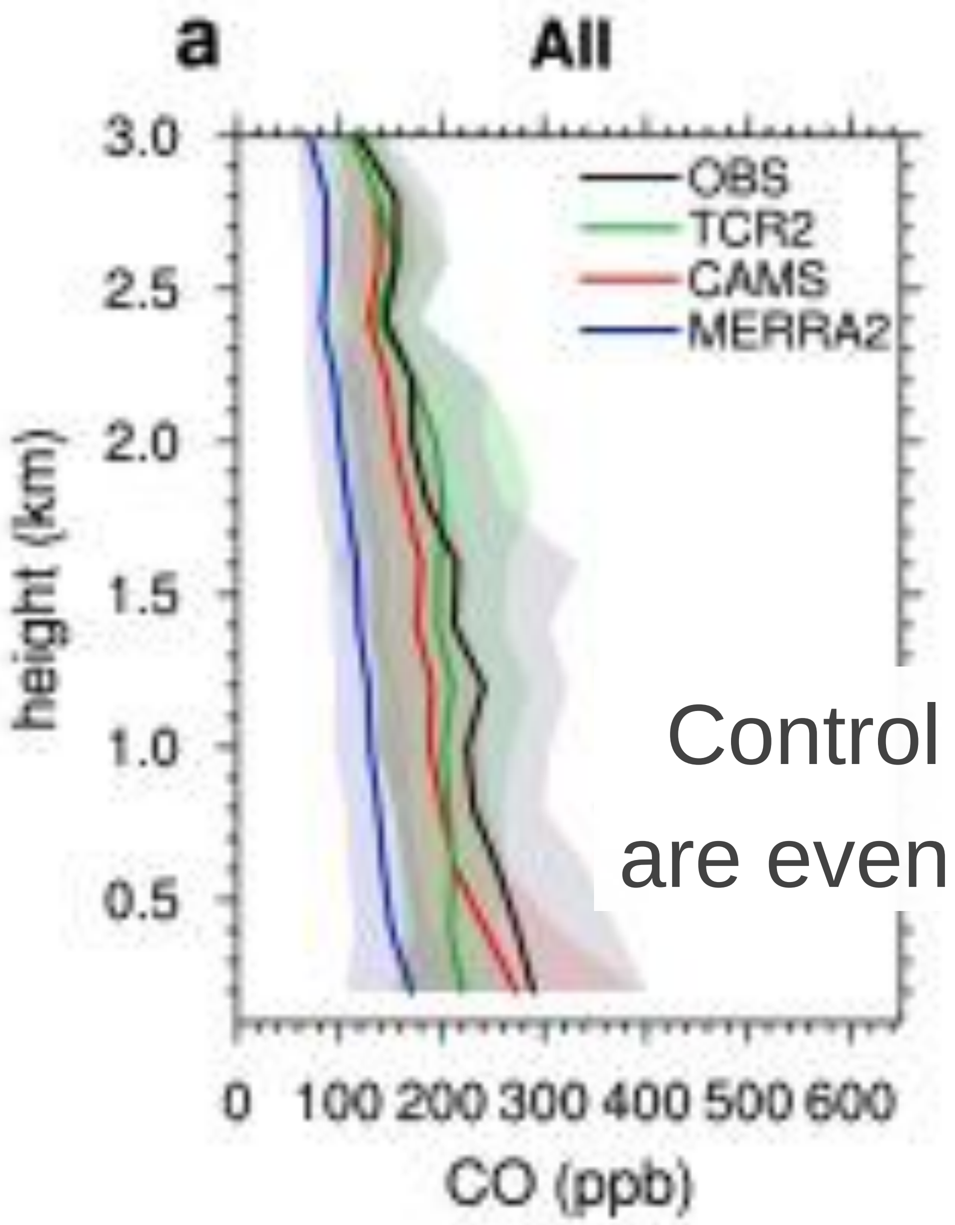
Park et al, 2020



The meteorological reanalysis needs to be improved substantially throughout the troposphere

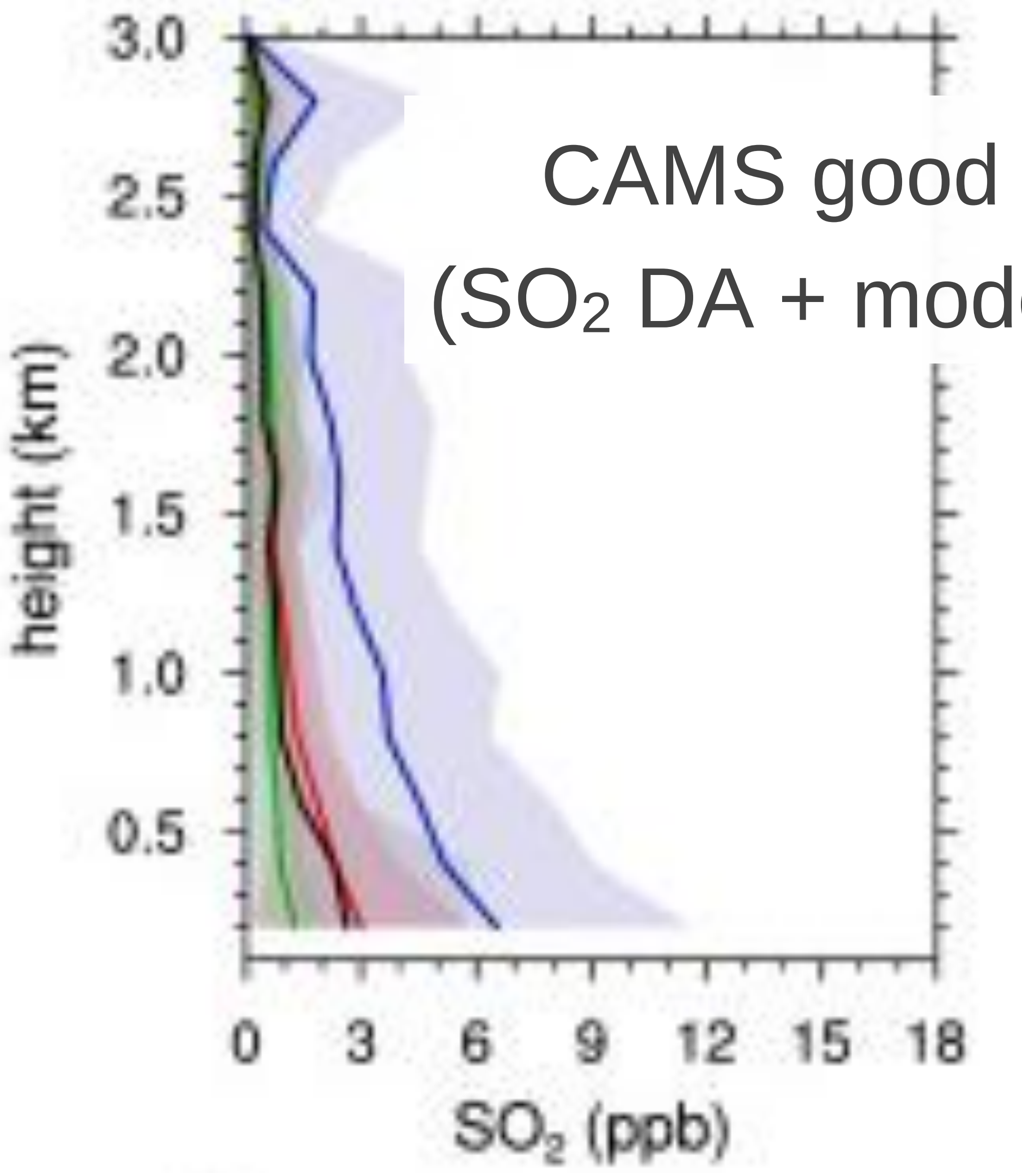
Chemical reanalysis inter-comparisons: Multi-species

CO



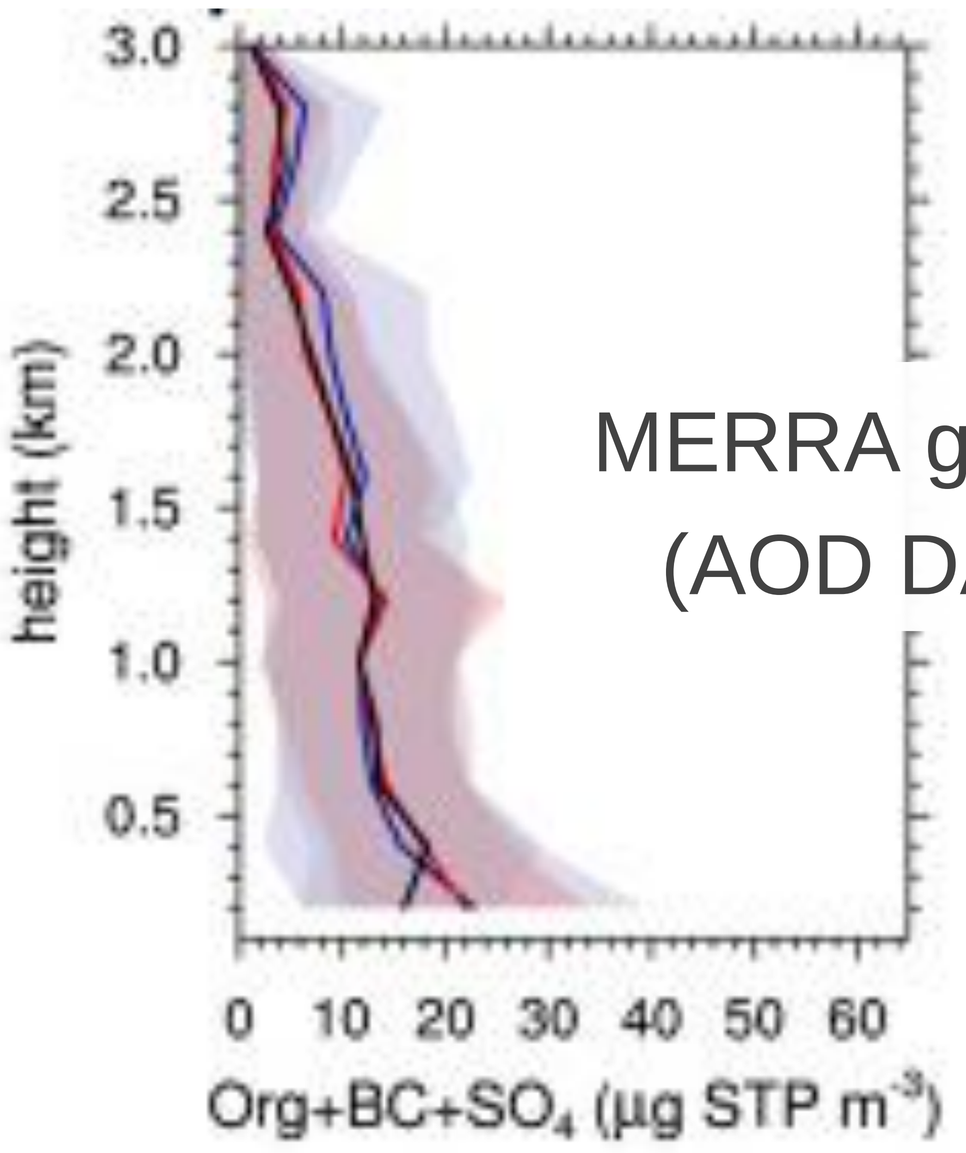
Control runs are even lower

SO_2



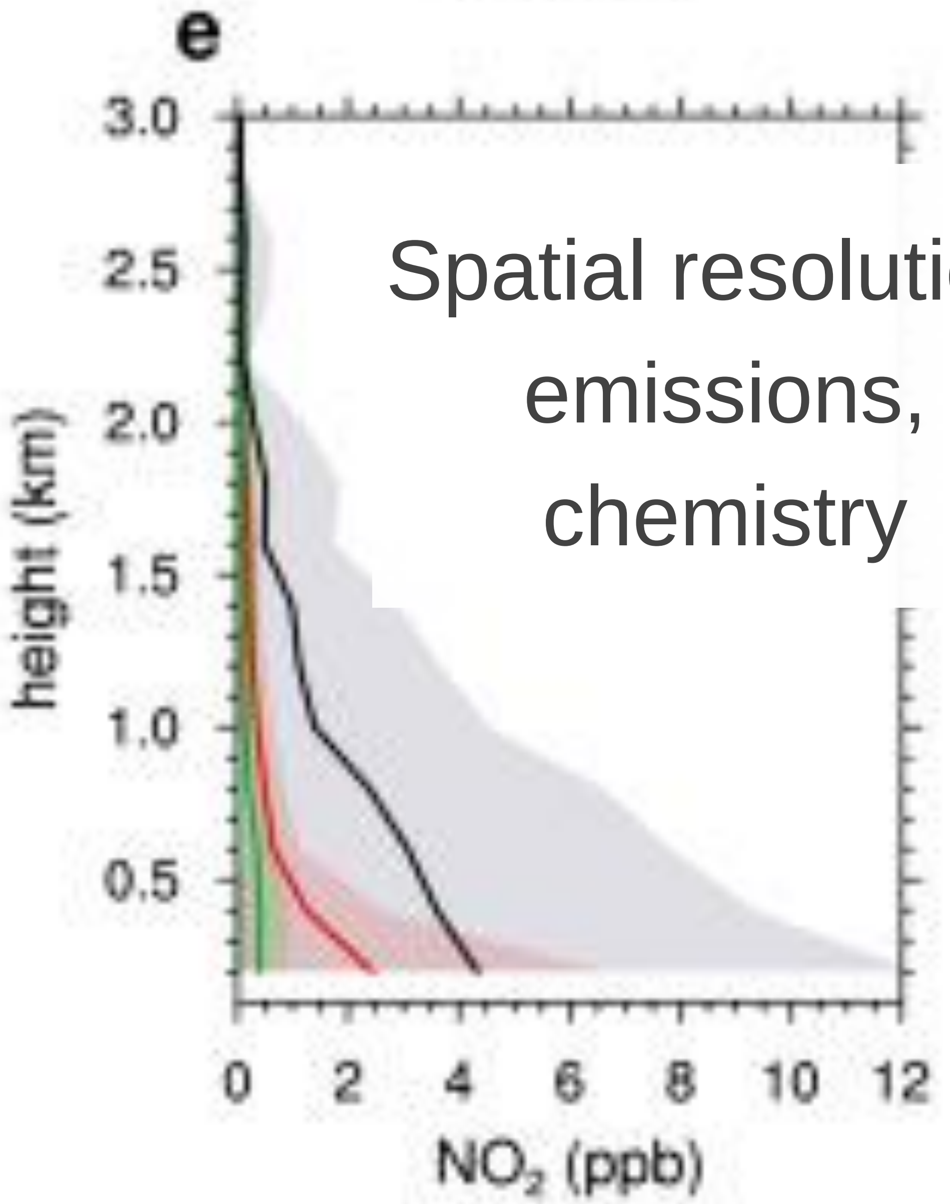
CAMS good
(SO_2 DA + model)

PM



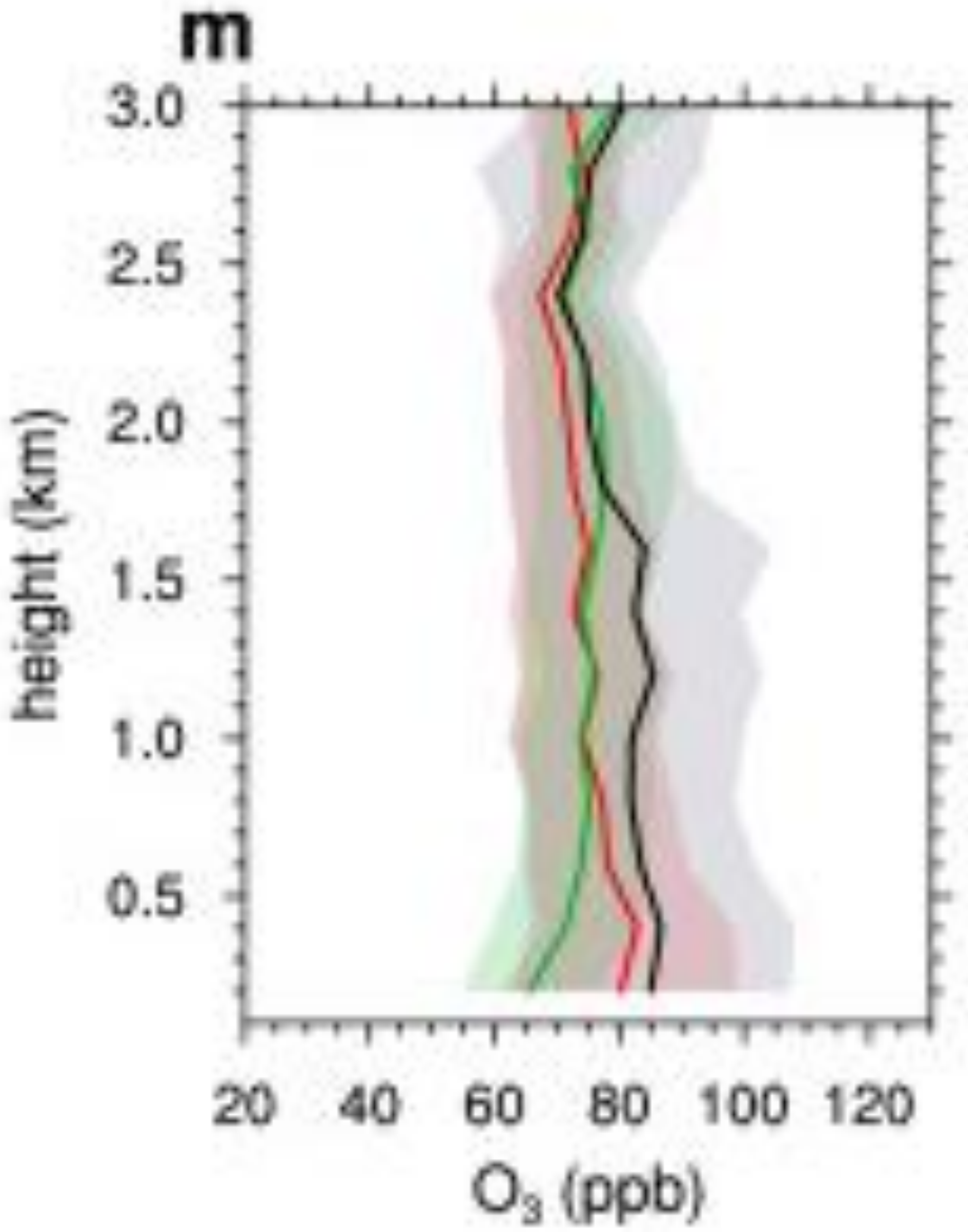
MERRA good
(AOD DA)

NO_2



Spatial resolution,
emissions,
chemistry

O_3



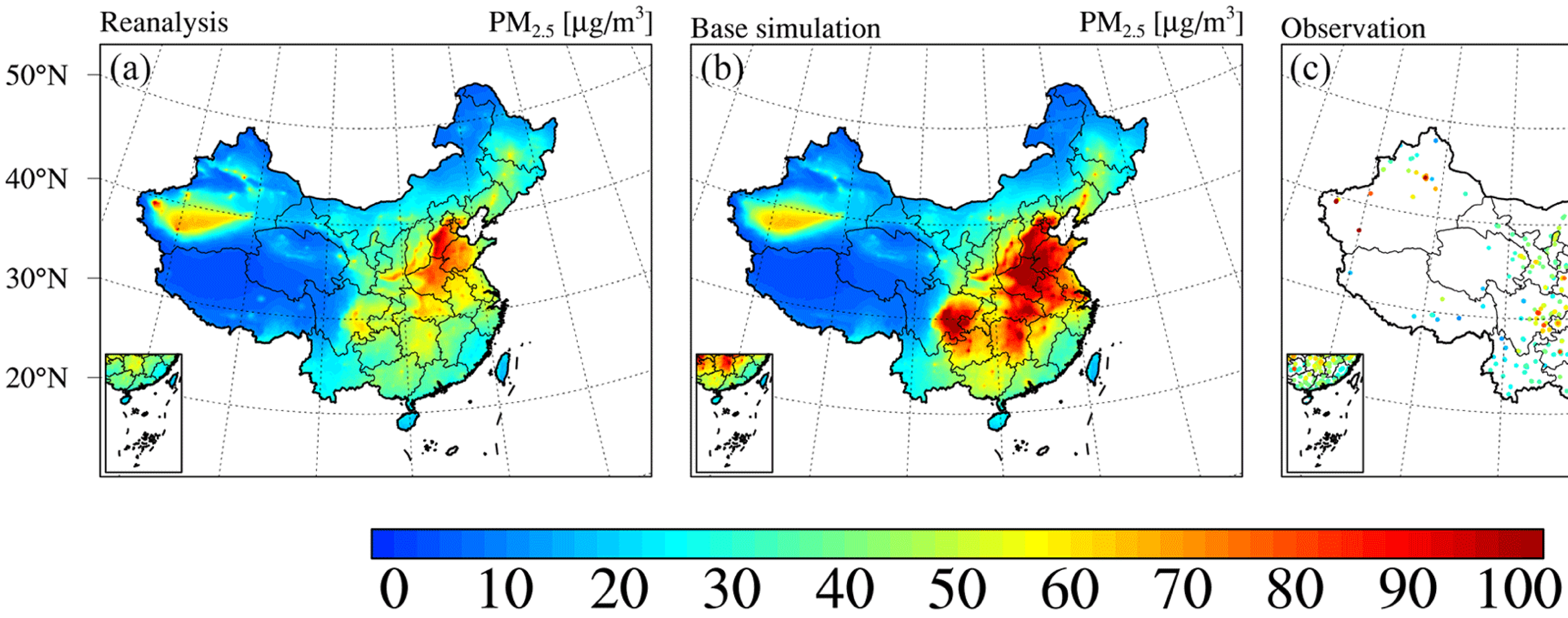
Multi-species validation over South Korea during KORUS-AQ campaign

Essential to improve precursors species to reproduce ozone

Ryu and Min, 2021

Regional chemical reanalysis

A 6-year high-resolution (15x15 km) Chinese air quality reanalysis (CAQRA) combining surface observations (PM2.5, PM10, SO_2, NO_2, CO, O_3)

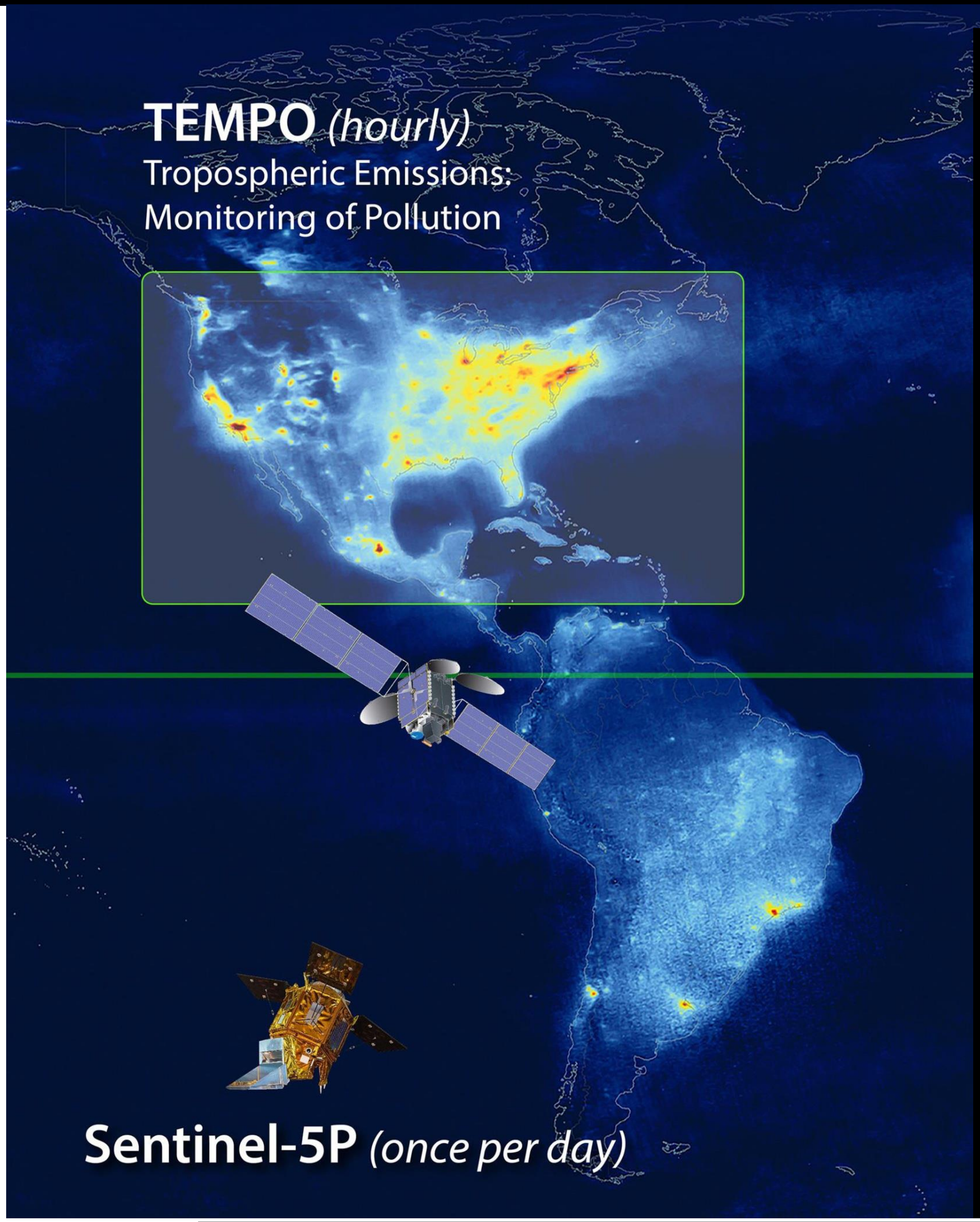


Kong et al, 2021

Regional high-resolution model + surface obs → local air quality

<u>*Challenges*</u>: representativeness, data quality, model resolution, combination with satellite data

Towards an Air Quality Constellation

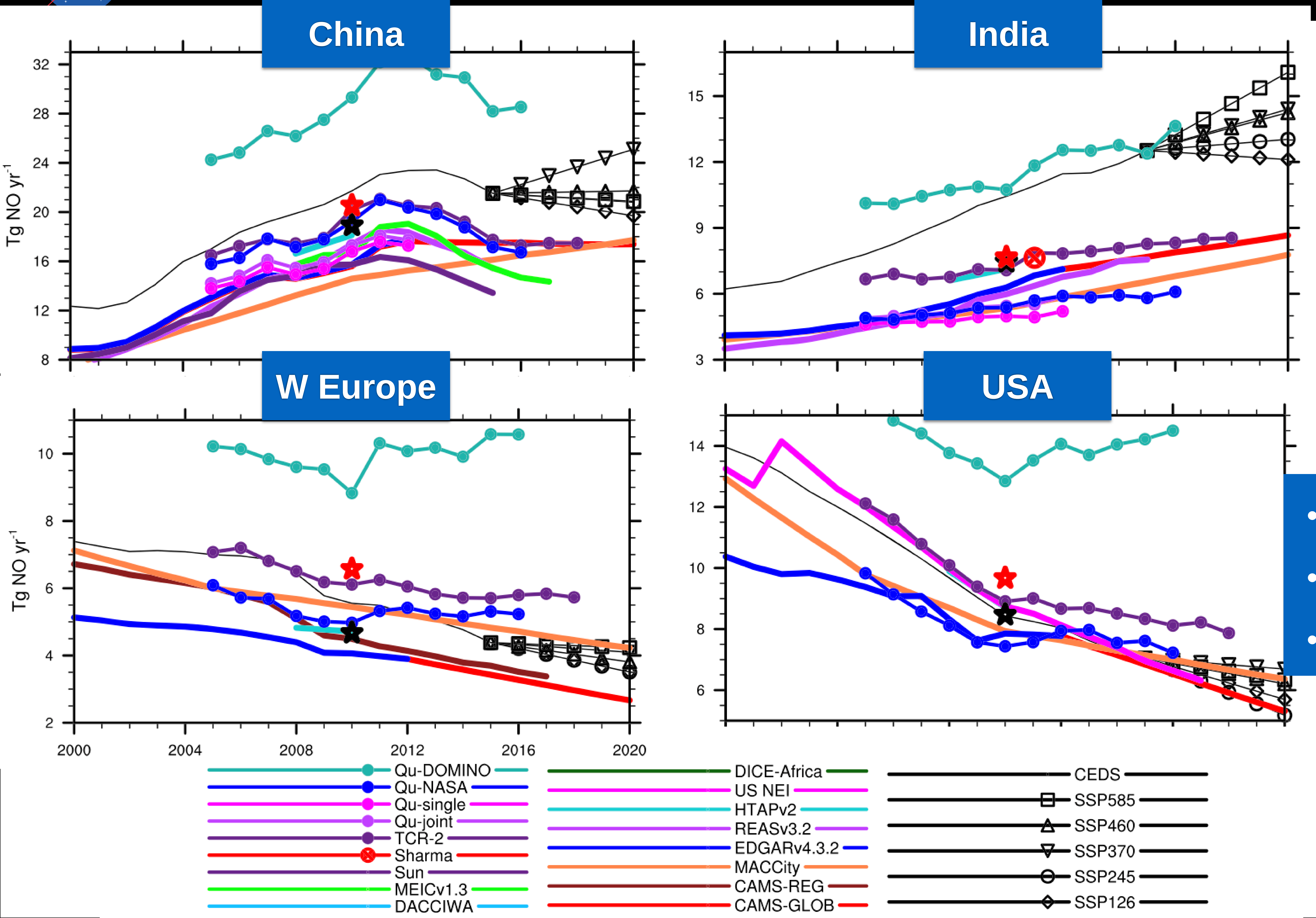


How does the constellation improve knowledge of global air quality?

- GEO sounders will provide an unprecedented number of composition observations at high spatial resolution.
- LEO sounders (IASI, CrIS, S5p) provide the global picture and thread the GEO observations together.

We face new challenges in integrating these different types of observations

Surface emissions in chemical reanalysis



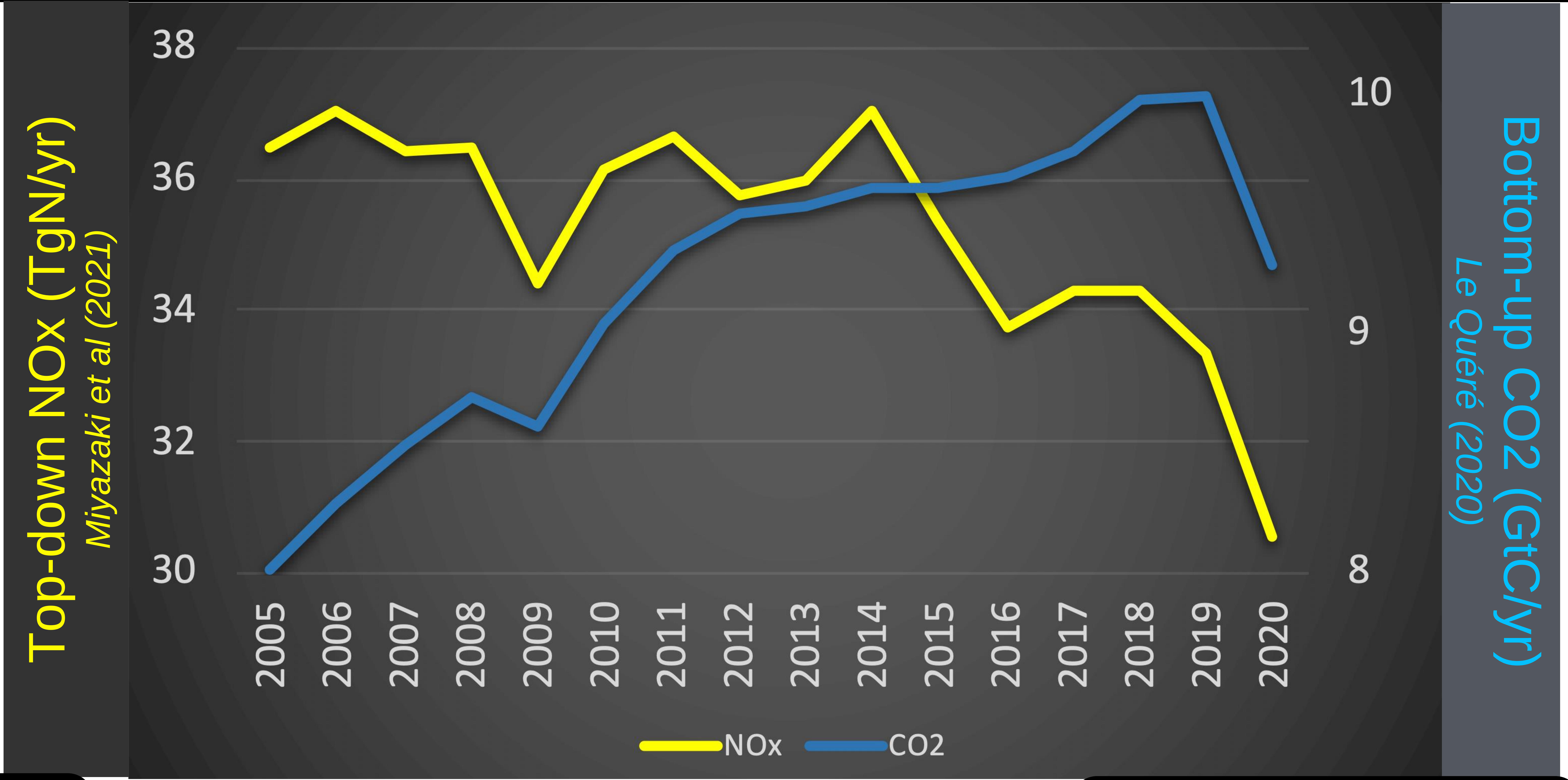
Emissions estimation from chemical reanalysis

↓

- Emission scenario evaluation
- Attribution study
- Environmental policy

Elguindi et al., 2020

Global anthropogenic emission reductions in 2020: 7% (CO_2) 8% (NOx)



1. Emissions (NOx, SO2, CO) → 2. Concentrations → 3. Health and climate Impacts

Jiang et al. 2020 ACP

Miyazaki et al. 2020 GRL

Miyazaki et al. 2021 Science Adv.

Laughner et al. 2021 PNAS

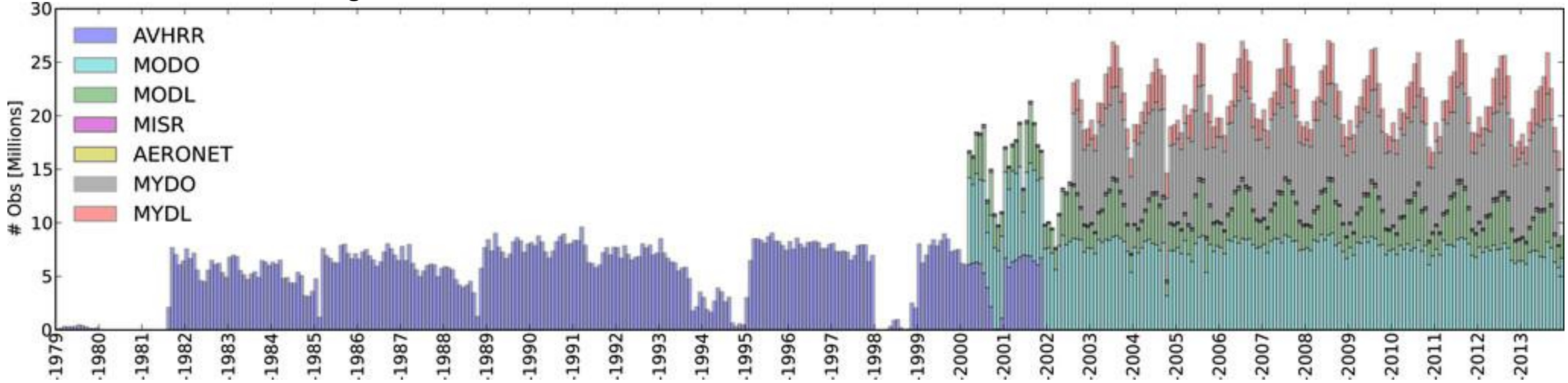
Sekiya et al. 2023 Science Adv.

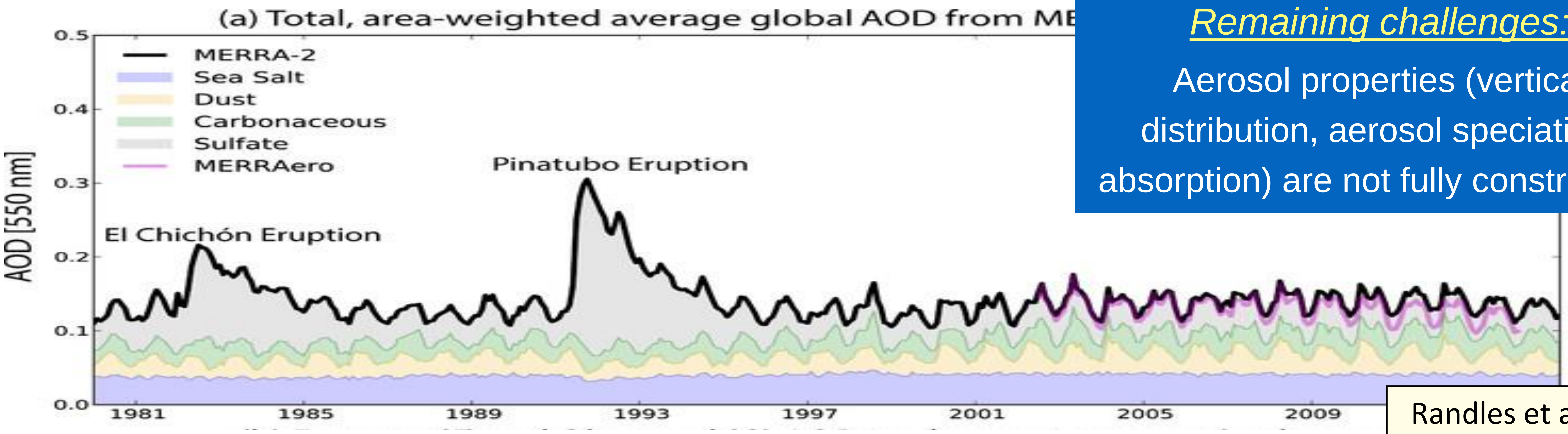
Stringency Index
100
80
60
40
20
0
Feb 2020
Mar 2020
Apr 2020
May 2020
Jun 2020
Jul 2020
Feb 10 2020
NOx Anomaly, kgN/m²s
-0.15
-0.075
0.0
0.075
0.15
-0.2
-0.1
0.0
0.1
0.2
-0.3
-0.15
0.0
0.15
0.3
United States
Italy
China

→ Better understand the efficacy of policies that co-benefit air quality and climate

MERRA-2 aerosol reanalysis

Total global number of observations from various AOD and aerosol observations





Remaining challenges:

Aerosol properties (vertical distribution, aerosol speciation, absorption) are not fully constrained.

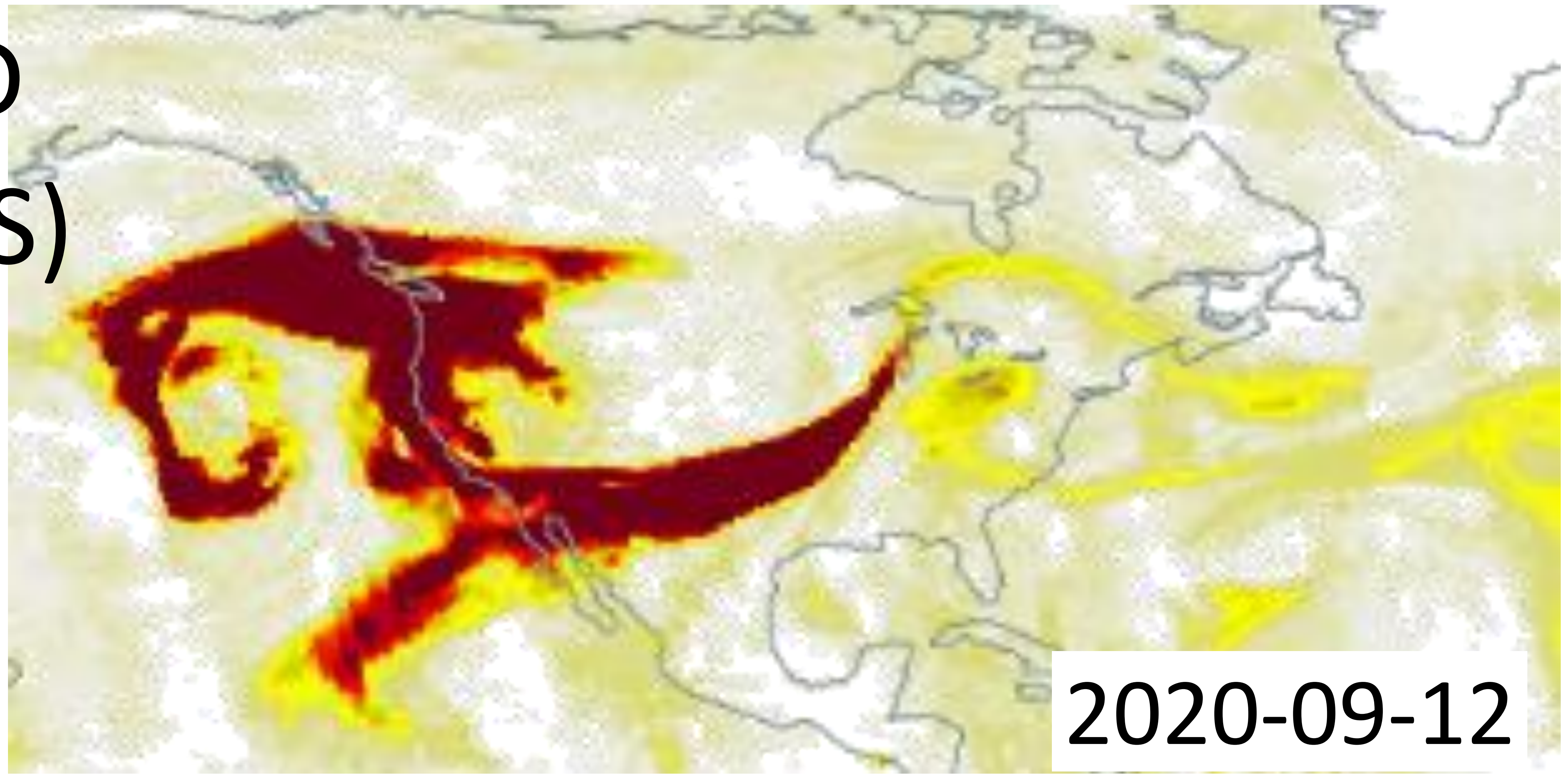
Randles et al, 2017

Sulfate, Nitrate, and Ammonium (SNA) aerosols

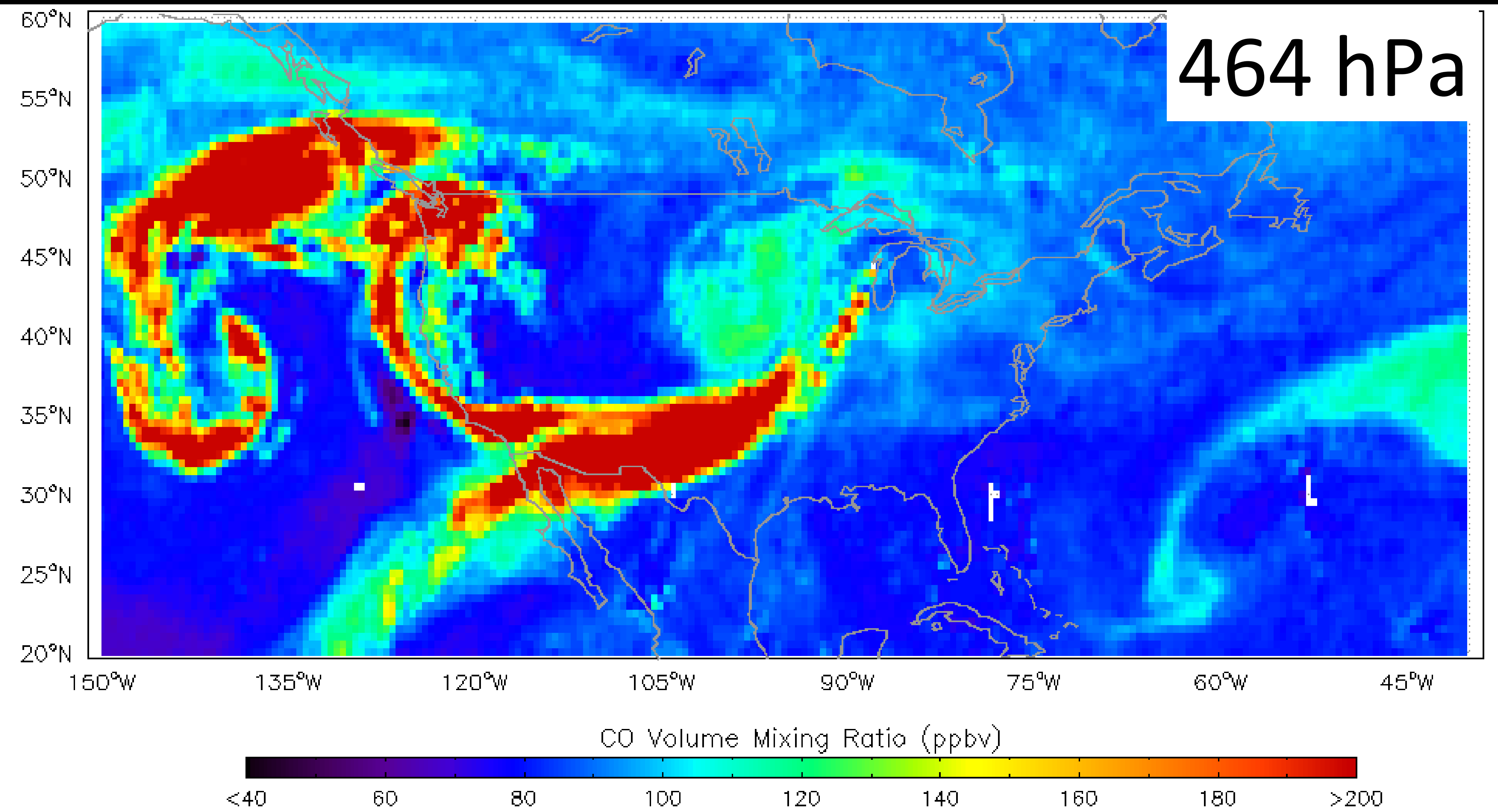
- Strong (10-20%) decreases in secondary inorganic aerosols due to COVID → + 0.14W/m2
- The obtained responses in emissions, aerosols, and climate forcing highlight the importance of aerosol & trace gas reanalysis in the climate impact assessment and Earth system reanalysis

CrIS composition data: 2020 California wildfires

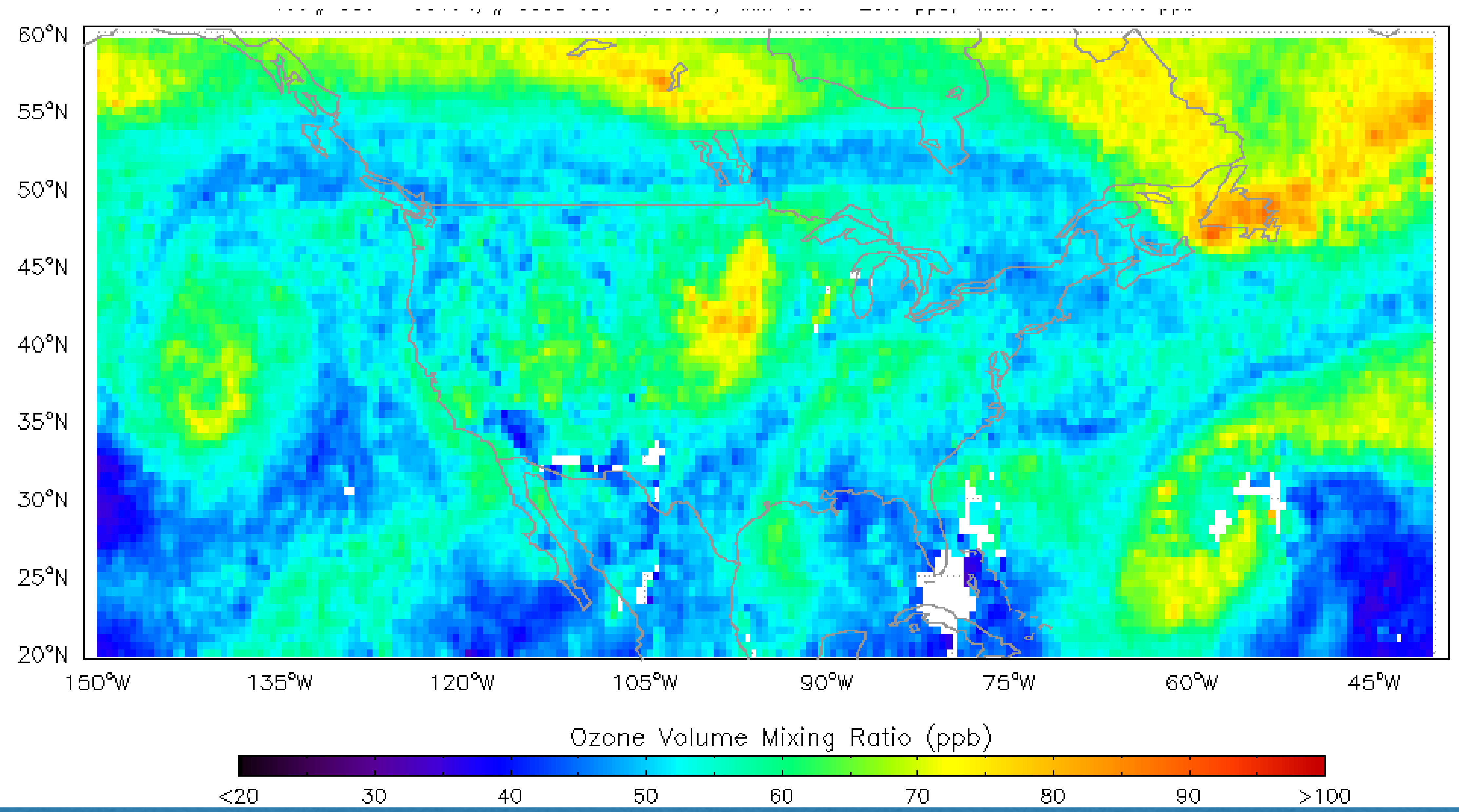
AOD (VIIRS)



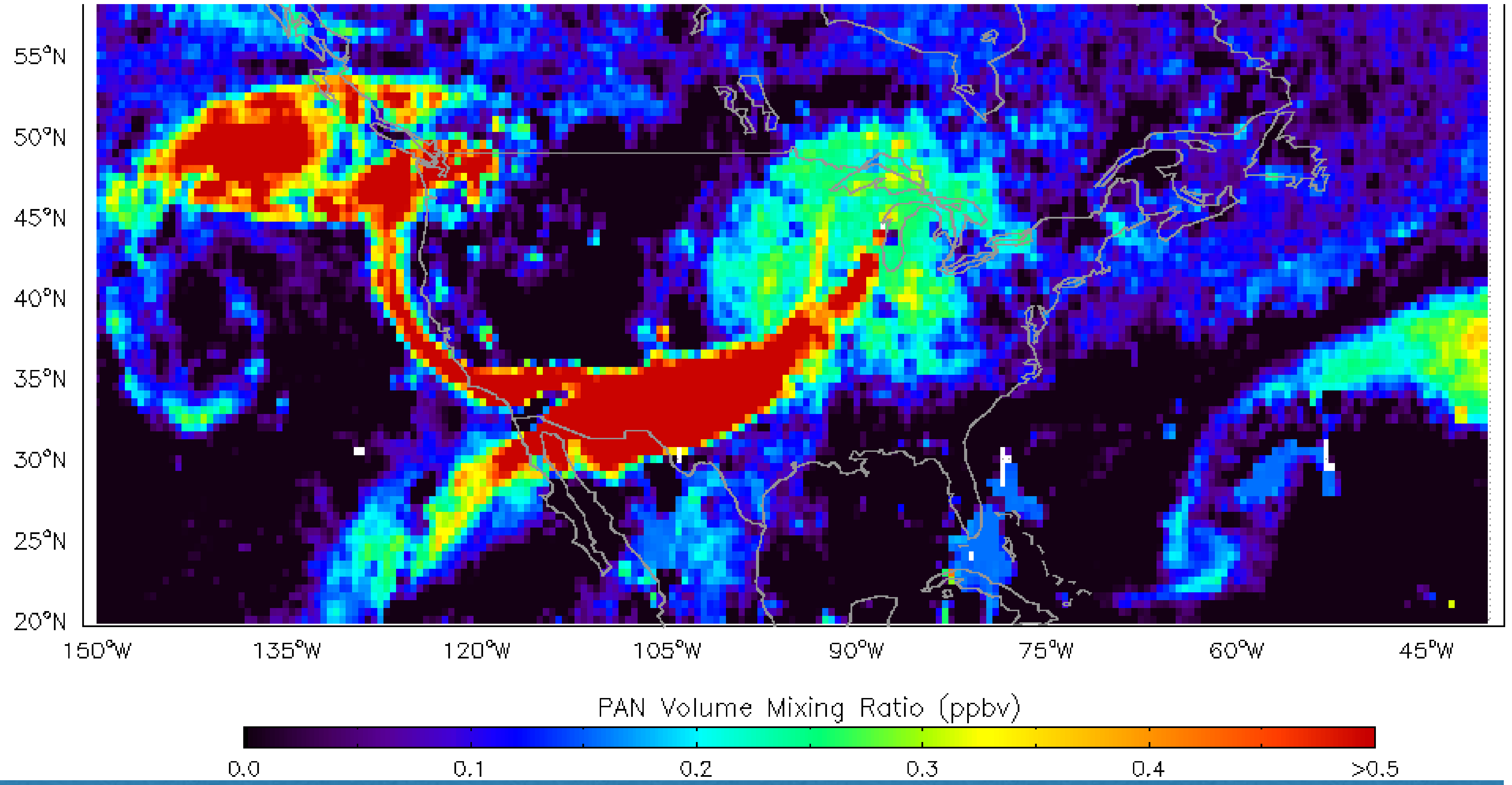
CO



O_3



PAN

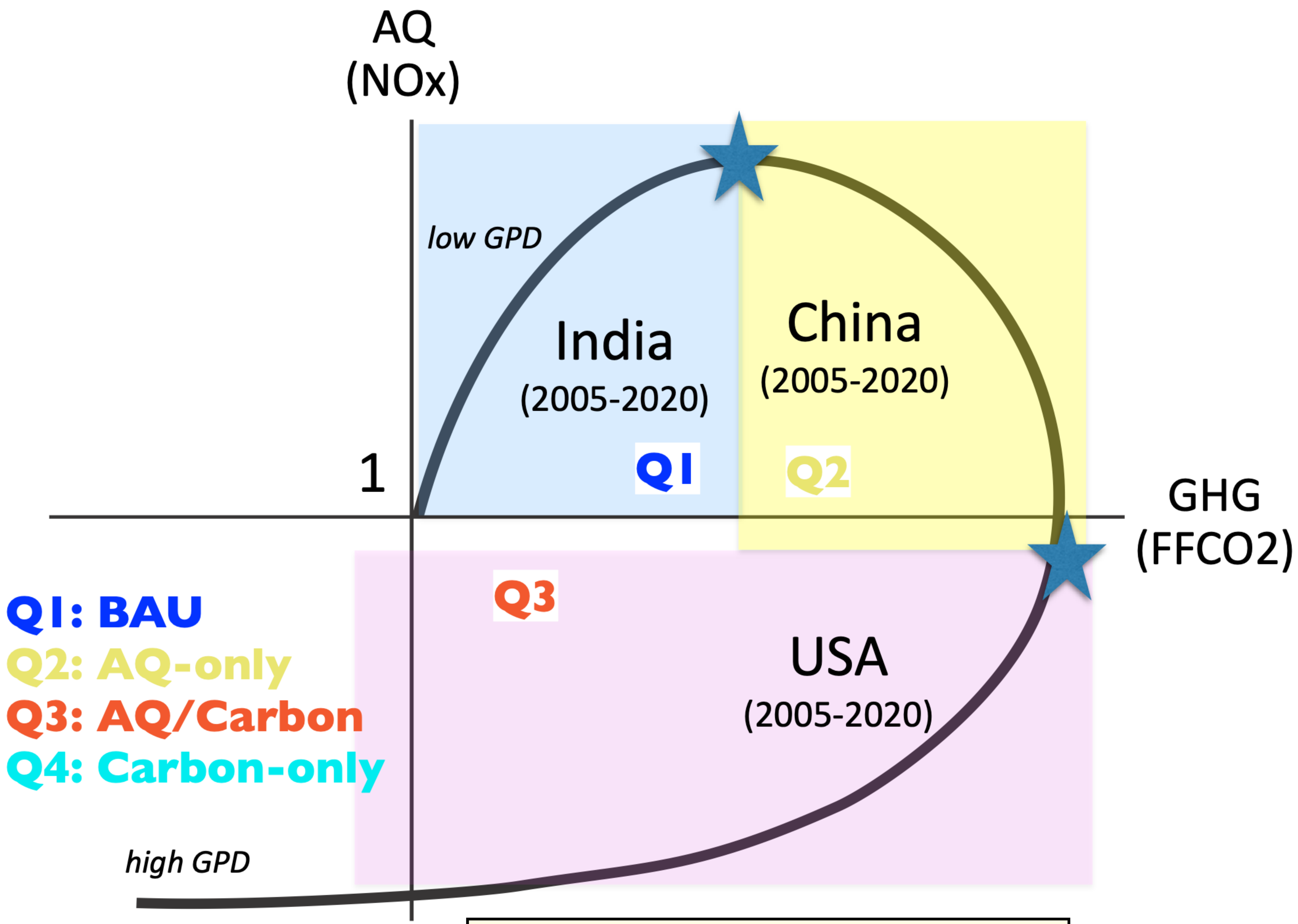


Assimilating CrIS data (+NH_3) will comprehend our understanding of source attributions

Estimation of fossil fuel CO_2 from chemical renalaysis emissions

From chemical reanalysis to carbon cycle and climate

- Quantifying the coevolution of GHG and AQ pollutants, associated with increased regulation and economic development, can provide insight into underlying anthropogenic processes.
- We classify the dynamics of historic emissions in terms of a modified Environmental Kuznets Curve (MEKC).
- The predictive skill of $FFCO_2$ less than 2% error at one-year lags and < 10% for 4-year lags.



Miyazaki and Bowman, Nature comm., 2023

<u>*GHG*</u>

Fossil fuel CO2 (FFCO2)

<u>*Air pollutants*</u>

Summary

- The chemical reanalysis data, combined with suborbital and ground-based measurements, has been used to improve our understanding of atmospheric composition and to evaluate new satellite data products.
- New LEO and GEO measurements and multi-spectral retrievals of composition provide much-improved spatial and temporal resolution and coverage in conjunction with the chemical reanalysis. They should lead to greater usefulness of satellite measurements for climate and air quality applications.
- Combining various Earth observations while accounting for interactions between trace gave, aerosols, and GHG is essential to understanding anthropogenic and natural influences on climate and for Earth system reanalysis.